

**The 1995 Atmospheric Trace Molecule Spectroscopy (ATMOS) Linelist**

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## Abstract

The Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment uses a Fourier transform spectrometer on board the space shuttle to record infrared solar occultation spectra of the atmosphere at 0.01 cm<sup>-1</sup> resolution. This article describes the current version of the molecular spectroscopic database used for the analysis of the data obtained during three Space Shuttle missions between 1992 and 1994. It is an extension of the effort first described by Brown et al., (Appl. Opt. 26, 5154-5182, 1987) to maintain an up-to-date database for the ATMOS experiment. The three-part ATMOS compilation contains line parameters of 49 molecular species between O. and 10000 cm<sup>-1</sup>. The main list with nearly 700,000 entries is an updated version of the HITRAN 1992 database. The second compilation contains supplemental line parameters, and the third set consists of absorption cross sections to represent the unresolvable features of heavy molecules. The differences between the ATMOS database and other public compilations are discussed.

## Introduction

The Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment records infrared solar occultation spectra of the atmosphere between 580 and 4800  $\text{cm}^{-1}$  at  $0.01\text{cm}^{-1}$  resolution using a Fourier transform spectrometer on board the Space Shuttle [1]. This instrument was first flown in 1985 on Spacelab 3. In 1992, 1993 and 1994, as part of the ATLAS 1,2 and 3 payloads, it obtained a more extensive set of spectral data for the  $69^{\circ}$  N to  $72^{\circ}$  S latitudes with tangent heights between 5 and 150 km including observations inside the remanent Arctic and Antarctic vortices [2]. These measurements were analyzed to obtain atmospheric pressure, temperature and volume mixing ratios as a function of the terrestrial co-ordinates. This article describes the comprehensive, customized catalog of molecular line parameters used for the version 2 analysis of the ATLAS series data and for reprocessing of the Spacelab 3 spectra.

An earlier version of the ATMOS molecular database was compiled in 1987 [3] and used for the initial analysis of ATMOS data obtained during the 1985 Spacelab 3 mission. The bulk of the parameters were placed in the main linelist and consisted of major modifications to the 1982 Air Force (icophysics Laboratory (AFGL) compilation [4,5]. A secondary list, called the Supplemental Linelist, was formed to include preliminary and lower quality data including parameters for the difficult-to-characterize species like the chlorofluorocarbons. In 1992, the ATMOS investigators set aside its 1987 main list and adopted the 1992 HITRAN database [6] since the public compilation contained most of the revisions needed by ATMOS. As with the 1987 linelists, the improvements in the main 1995 ATMOS database were made, in the 580 to 4800  $\text{cm}^{-1}$  region using recent laboratory data as well as parameters from the 1991 GEISA compilation [7]. The ATMOS supplemental list was also changed by the removal of artificial line parameters created previously [3] from room temperature cross sections so that new experimental temperature-and (sometimes) pressure-dependent absorption coefficients could be used for some heavy species. For the 1995 update, a third list was initiated using available experimental absorption cross section files [8-19]. The philosophy of having three separate lists is so that the one (main) list consists of generally valid parameters based on published studies, another (supplemental) is the depository of approximate predictions and the third list contains empirical absorption coefficients. In contrast to the first

ATMOS compilations [3], few unpublished studies have been included in the 1995 version. An overview of the linelists is given in **Table 1** by showing the ATMOS molecule number, species(MOLECULE), total number of transitions (#LINES), the minimum and maximum ranges( $\nu_{\text{MIN}}, \nu_{\text{MAX}}$ ) in wavenumber( $\text{cm}^{-1}$ ), followed by the number of isotopes (# ISO), vibrational states (#VIB) and bands (#BANDS) and the total integrated absorption in  $\text{cm}^{-1}/(\text{molecule}\cdot\text{cm}^2)$  at 296 K. Those parameters marked by “s” to the left of the molecule number appear in the supplemental list while those marked by “c” are available in cross section files. Some species appear in more than one linelist, but, with the exception of the overlapping lists of  $\text{CHClF}_2$  (WC-22) cross sections, no spectral band of any species is duplicated in order that all three lists can be used simultaneously.

### General Description of the ATMOS Linelists

The main and supplemental ATMOS lists contain the same type of molecular parameters as the 1992 HITRAN database, but the format is slightly different. A sample section of the 1995 ATMOS main and supplemental linelist is shown in **Table 2** with the name of the molecule given in the first column. The parameters include molecule and isotope code numbers, positions in  $\text{cm}^{-1}$ , intensities in  $\text{cm}^{-1}/(\text{molecule}\cdot\text{cm}^2)$  at 296 K, lower state energies in  $\text{cm}^{-1}$  air-broadening and self-broadening coefficients in  $\text{cm}^{-1}/\text{atm}$  at 296 K, the transition matrix element(r2), the temperature dependence exponent of the air-broadening coefficients n, and the air-broadened pressure shifts in  $\text{cm}^{-1}/\text{atm}$  at 296 K. These are followed by the upper and lower vibrational state index codes ( $V_{\text{UP}}$  and  $V_{\text{LO}}$ ), rotational quantum numbers, and the accuracy and reference codes integers.

To summarize the isotopic nomenclature, **Table 3** gives the molecule number, species, isotope numbers, the old isotopic codes used prior to 1986 in the AFGL compilations [4,5], the chemical formula and the assumed isotopic abundances.

The upper and lower state vibration index codes in Table 2 can be translated into corresponding standard vibrational nomenclature using software like those in the FORTRAN program "SHELLCI" given on the 1992 HITRAN compilation. Table 4 displays the integer codes for  $V_{\text{UP}}$  and  $V_{\text{LO}}$  in Table 2 with their corresponding vibrational quantum numbers. The index is usually incremented in order of increasing energy so that “1” is the ground state ( i.e. 000 for  $\text{H}_2\text{O}$  or 00001 for C(), or X0 for O,); “2” is the lowest fundamental; and “3” is the

next higher state (an overtone or fundamental). The molecules all fall into one of ten groups, **Diatomics** are in Groups 4,6 and 7. Species with three atoms are contained in Group 1 (asymmetric rotors), Group 8 (symmetric rotors) and Groups 2 and 3 (linear molecules). Molecules with four atoms are in Groups 9 and 10. Group 5 was originally setup for the spherical rotors like  $\text{CH}_4$ , but it has become the catch-all group for species with five or more atoms, regardless of molecule symmetry. For Group 5, the ground state of the non-spherical species has an index of “14.” Thus in **Table 2** the vibrational indices of “27 14 for the  $\text{CH}_3\text{Br}$  line at 971.2295 cm<sup>-1</sup> should be interpreted as transitions of the  $\nu_3$  band from the ground state.

The accuracy and reference codes [ace and rcf in Table 2] are two sets of three integers each that respectively indicate the estimated uncertainties and data sources for the positions, intensities and air-broadening coefficients. The error codes defined by Rothman et al. [6] and used by **ATMOS** are given in **Table 5**. For example, a code of “564” means that the accuracies are between 0.00001 and 0.0001 cm<sup>-1</sup> for positions, between 2 and 5% for intensities and from 10 to 20% for air-broadening coefficients. Reference number fields defined for the 1992 HITRAN linelist give the index of references that correspond to a list distributed electronically with the 1992 HITRAN edition. The publications are grouped by molecule and separated into three sub-groups that are numbered individually for positions, intensities and line widths. The code “O O O” means that the entry was the same in 1986 [8] while a code “2 3 4” means that the positions are based on reference 2 of the first subset, intensities on number 3 of the second subset and widths on number 4 of the third group listed for water. In changing the **ATMOS** linelist, an attempt has been made to be consistent with the 1992 numbering scheme by incrementing the counter for each new study. However, the reference codes for the new bands in the 1995 **ATMOS** list will not be consistent with the codes expected on the 1995 HITRAN database because the two databases will be different. In addition, these fields are usually not defined in the supplemental list, as seen in Table 2 for the  $\text{CH}_3\text{I}$  and  $\text{CH}_3\text{Br}$  transitions.

One difference between **ATMOS** and the two public databases (HITRAN and GEISA) is the molecule code number. The **ATMOS** number codes for 46 molecules were specified in 1982 to match evolving software at a time when the public databases contained 21 species. As a result, while molecules 1 -20 have the same codes on both the **ATMOS** and HITRAN databases, all the molecules codes are different between 21-50. The

correspondence of the numbering schemes between the three compilations is shown in **Table 6**. The isotope codes are generally the same as the other two databases. One exception is HDO which is labelled in the ATMOS database as a separate molecule (49) rather than the minor isotope of molecule 1 (water). In addition, parameters of PH<sub>3</sub> are omitted entirely from the ATM OS linelist, and no parameters are currently included for C<sub>2</sub>H<sub>4</sub>(molecule 39).

### Absorption Coefficients

Line parameters are difficult to obtain for important atmospheric species such as the chlorofluorocarbons and N<sub>2</sub>O<sub>5</sub>. As an alternative, the remote sensing community has often relied on absorption coefficient (or cross section) parameters. In the mid-1980's, the work of Massie et al.[9] provided cross sections from pure gas laboratory spectra at room temperature. By scaling these coefficients by the grid spacing (cm<sup>-1</sup>/ point value), ATMOS transformed some of these into "pseudo-line" parameters for the supplemental list [3] that could be used in the "line-by-line" calculations of the forward models within the ATMOS software. This type of transformation also permitted pressure-broadening coefficients to be applied. Later, new pure gas spectra were obtained for a range of atmospheric temperatures by McDaniel et al. [10] and Cantrell et al. [11] so that a total of fourteen heavy species could be included in the 1992 HITRAN compilation [6,12]. While these older results can be employed for ATMOS calculations, only the N<sub>2</sub>O<sub>5</sub> parameters from Cantrell et al. [11] and part of the CFC-22 parameters from McDaniel et al. [10] are being used since newer studies [13-19] are available. The current parameters that dominate ATMOS retrievals of eight heavy species are summarized in **Table 7** by showing the reference, spectral range, experimental temperatures and total gas pressures, the integrated intensities and data grid spacing (cm<sup>-1</sup>/point). For CCl<sub>4</sub>, the new temperature-dependent parameters of Orlando et al. [13] are utilized. For CFC-11, CFC-12, SF<sub>6</sub> and the dominant part of a CFC-22 feature, more recent cross sections were obtained [14-17] from laboratory spectra of the gases broadened by nitrogen at gas pressures and temperatures that correspond to the terrestrial atmosphere [20]. For CCl<sub>3</sub>F(CFC-11), cross sections for the 850 cm<sup>-1</sup> band reported by Li and Varanasi [14] are used. For the 922 cm<sup>-1</sup> band of CCl<sub>2</sub>F<sub>2</sub>(CFC-12), the work of Varanasi and Nemtchinov [15,16] is included. In the case of CHCl<sub>2</sub>F(CFC-22), the very high resolution laser data from

Varanasi [17,18] is utilized for the peak of the  $2\nu_2$  Q-branch at  $829\text{ cm}^{-1}$  while the lower resolution data from McDaniel et al. [10,12] are added to characterize the other portions of the band. Finally, the absorption coefficients at 200K reported by May and Friedl [19] are used for the  $\text{HO}_2\text{NO}_2$  band at  $803\text{ cm}^{-1}$ . Several decisions were required in order to use these cross sections with the ATMOS analysis software. For example, interpolations to specific atmospheric pressures and temperatures are usually done as a function of temperature for most of the species, except for the peak absorption of  $\text{CHClF}_2$ , where interpolation is done by log (pressure). If several pressures are available at a single temperature then the data for the lowest pressure is selected. For temperatures beyond the range of the laboratory data, no extrapolations are done, and laboratory cross section data nearest the desired temperature is used. Fits to ATMOS ATLAS 3 spectra are illustrated in Fig. 1. The top panel shows the CFC-12( $\text{CCl}_2\text{F}_2$ ) band at  $924\text{ cm}^{-1}$ . The P branch region is too overlapped by  $\text{HNO}_3$  transitions to be included in the retrieval interval. In addition, the wavenumber calibration of the CFC-12 absorption coefficients was increased by  $0.002\text{ cm}^{-1}$  to align the Q branch features with the stronger  $\text{CO}_2$  transitions appearing in the R branch. The bottom panel shows the CFC-11 ( $\text{CCl}_3\text{F}$ ) band at  $849\text{ cm}^{-1}$ . The sharp peaks between  $856$  and  $870\text{ cm}^{-1}$  arise from  $\text{HNO}_3$  while the structure between  $830$  and  $850\text{ cm}^{-1}$  are due to  $\text{CO}_2$  and  $\text{O}_3$ . For CFC-11, no wavenumber adjustment has been applied. It is emphasized that the content of the absorption coefficient database is continually changing. For example, the new data of Newnham et al. [21] for the room temperature data for  $\text{N}_2\text{O}_5$ , the Menoux et al. study [22] for collision-induced  $\text{N}_2\text{-N}_2$  and  $\text{N}_2\text{-O}_2$  and the temperature-dependent and pressure-broadened cross sections of  $\text{CF}_4$  [23] and  $\text{CHCl}_2\text{F}$  [18] from Varanasi are being considered for future revisions.

### Alterations to Molecular Line Parameters

The following sections discuss the modifications made to the 199211 ITRAN database and the 1987 ATMOS supplemental linelist to create the 1995 ATMOS compilations. **Table 8** gives an overview of the available studies [24-14] which were incorporated by showing the species, the region or band which were modified according to positions v, intensities I or air-broadened widths  $\gamma$ . More detailed summaries of the resulting parameters in **Tables 9** and **10** list the molecule numbers in parentheses, vibrational bands, isotope

number, the number of lines (#LINES), the minimum and maximum wavenumber ranges covered (FMIN,FMAX), minimum and maximum intensity ranges (IMIN,IMAX), the sum of the intensities (S-SUM) in  $\text{cm}^{-1}/(\text{molecule}\cdot\text{cm}^2)$  at 296 K, the accuracy and references codes. The tables also show the minimum and maximum values of air-broadened halfwidths (PBIIW,PMAX), self-broadened halfwidths (SELF,SMAX), and the temperature dependence coefficient of the air-broadened widths n (NTDP,NMAX). Since most of the pressure shifts are set to zero, these are not included in Table 9 and 10. The temperature dependence coefficient is used to compute the expected linewidth using Eq. [1]

$$\gamma(P,T) = \gamma_o(P_0, T_0 = 296\text{K}) \cdot (296/T)^n \cdot P \quad \text{Eq. 1}$$

where  $\gamma_o$  is the half-width in  $\text{cm}^{-1}/\text{atm}$  at  $T = 296\text{ K}$  and  $P$  is pressure in atm. Table 9 gives data for only the modified species in the main ATMOS linelist, while Table 10 summarizes all the species presently on the supplemental list. Complete summaries of the database can be obtained from the first author. The individual modifications are described below in order of molecular number. Entries for  $\text{H}_2\text{CO}$ ,  $\text{HONO}$ ,  $\text{CH}_3\text{F}$ ,  $\text{CH}_3\text{CCl}_3$ ,  $\text{CH}_3\text{Br}$ ,  $\text{CH}_3\text{I}$  and  $\text{Cl IFCl}_2$  in the supplemental list have not changed and are described in the 1987 article [3].

## **H<sub>2</sub>O (1)**

Two changes were made to the water parameters. In the 10  $\mu\text{m}$  region, 39 experimental intensities and 81 air-broadened linewidths from Rinsland et al. [24] replaced some of the calculated values for the stronger rotational and  $\nu_2$  transitions from 800 to 1100  $\text{cm}^{-1}$ . At 3  $\mu\text{m}$ , measured intensities of Toth [25] from 3003 to 4260  $\text{cm}^{-1}$  were used for 542 transitions of the  $2\nu_2$  band of the main isotope. Because only some of the transitions were replaced, the reference codes shown in Table 9 correspond to the unchanged lines. The reference codes for the altered features are 011111 and 770, respectively. Other recent measurements of Toth [26,27] have not yet been included.

## **O<sub>3</sub> (3)**

The ozone parameters were updated significantly for the 199211 ITRAN list [28]. For the updated ATMOS main list, some bands were revised and new entries were added for 36 bands to extend the ozone

catalog 104060 cm<sup>-1</sup>. The (004) and (310) bands at 2.5  $\mu\text{m}$  and the (103) band at 2.7  $\mu\text{m}$  were included [29,30]. At 3.4  $\mu\text{m}$ , eight hot bands were added between 2841 and 3102  $\text{cm}^{-1}$  [31]. At 5.5  $\mu\text{m}$ , the  $3\nu_3 - \nu_1$  hot band was revised, and at 10  $\mu\text{m}$ , several hot bands were merged [32]. At 17  $\mu\text{m}$ , calculated  $\nu_2$  parameters for  $^{16}\text{O}^{16}\text{O}^{17}\text{O}$  and  $^{16}\text{O}^{17}\text{O}^{16}\text{O}$  were incorporated [33]. However, the scaling of all ozone intensities by some 5% as inferred from the measurements of Pickett et al. [34] has been deferred until after confirmation by other investigators. The reference and accuracy codes of the altered transitions are indicated in Table 9. Some more recent studies [35-38] have not been included.

#### **N<sub>2</sub>O (4)**

The previous nitrous oxide on all the databases were either old predictions from the 1982 AFGL tape [5] for the 500-727 and 3293 to 5131 cm<sup>-1</sup> regions or a composite list prepared by Toth [39] in 1985 for the 894-2839  $\text{cm}^{-1}$  interval. For the 1995 ATMOS linelist, transitions between 3046 and 3493  $\text{cm}^{-1}$  were revised by replacing 6 existing bands and adding 26 missing bands using the work of Toth [40]. Modified entries are listed with reference codes of 11 1.

#### **CH<sub>3</sub>D (6)**

The intensities of the CH<sub>3</sub>D triad of  $\nu_6$ ,  $\nu_3$  and  $\nu_5$  between 970 and 1693  $\text{cm}^{-1}$  were recalculated to include the intensities results of Tarrago et al. [41]. The air-broadened widths were set to 0.08  $\text{cm}^{-1}/\text{atm}$  and the self-broadened to 0.09  $\text{cm}^{-1}/\text{atm}$ . The CH<sub>3</sub>D parameters in the 3.3  $\mu\text{m}$  region which are used for ATMOS retrievals have not been revised since 1982, however. The intensity measurements of five  $\nu_4$  lines reported by Rinsland et al. [42] have not been included in the expectation that an ongoing study [43] will provide a global revision of the 3.3  $\mu\text{m}$  CH<sub>3</sub>D.

#### **O<sub>2</sub> (7)**

Predictions of the 6  $\mu\text{m}$  transitions arising from the electric quadrupole and magnetic dipole were added, respectively, to the main [44] and supplemental [45] lists with air- and self- broadened coefficients set to 0.042 and 0.065  $\text{cm}^{-1}/\text{atm}$ , respectively. A constant value of 0.75 is used for the air-broadened widths temperature

coefficient.

#### NO (8)

The positions and intensities of the 1-0 band and the widths of infrared transitions were modified using the work of Spencer et al. [46]. The new line positions are systematically lower compared to the 1992 values: from 0.0003 cm<sup>-1</sup> at low J and to 0.001 cm<sup>-1</sup> at J = 22. The new intensities of the P and R branches are 3.6% higher between P13.5 and R 19.5, but the Q branch transitions and the higher m P and R branch lines are 8% lower compared to the 1992 HITRAN values [6]. Since air- and O<sub>2</sub> measurements are not generally available, the line widths are N<sub>2</sub>-broadening coefficients values from Spencer et al. [46]. The temperature dependence of the widths was set to a constant 0.71. The new measurements are only 1 to 4% different from the prior Ballard et al. results [47] that were used in the 1992 HITRAN update.

#### NO<sub>2</sub> (10)

The 6 μm region was revised for the 1538 to 1640 cm<sup>-1</sup> interval by replacing an older prediction in the 1992 HITRAN with an experimental linelist from Toth [48] that included transitions of v<sub>3</sub>, 2v<sub>2</sub> and v<sub>3</sub>-v<sub>2</sub>. Line widths were set to the default values on HITRAN of γ<sub>air</sub> = 0.067 cm<sup>-1</sup>/atm, γ<sub>eff</sub> = 0.0, and the temperature coefficient = 0.75, based on the work of Devi et al. [49] and May and Webster [50]. The reference codes for these changes are 441. The more recent work of Perrin et al. [51,52] has not yet been incorporated.

#### INO<sub>3</sub> (12)

The bands near 11 and 7.5 μm were revised substantially. In the first region, the prediction of the v<sub>5</sub>, 2v<sub>9</sub> parameters of Perrin et al. [53,54] replaced the line positions and relative intensities by Maki and Wells [55]. Approximate parameters for the 11 μm hot bands [56] were moved to the supplemental linelist. The intensities of the v<sub>5</sub> and 2v<sub>9</sub> near 900 cm<sup>-1</sup>, and v<sub>4</sub> and v<sub>3</sub> near 1300 cm<sup>-1</sup> were renormalized using Goldman et al. and Giver et al. [57,58], unpublished laboratory data, and ATMOS atmospheric data. There are considerable differences in absolute intensity studies; for the interim, it is thought that the normalization selected here sets the relative

band intensities to within  $\pm 10\%$ , but the absolute uncertainties for the integrated band intensities may be 10 to 15%. The relative intensities within bands may also vary by more than 20% in many cases. The air-broadened widths of  $0.11 \text{ cm}^{-1}/\text{atm}$  and a temperature coefficient of  $n = 0.75$  has been taken from May and Webster [59]. The recent results for the hot bands have not been included [60].

Analysis of the ATMOS atmospheric spectral data encompassing both the  $\nu_2$  and  $\nu_5$  bands revealed a systematic bias between the profiles retrieved from individual  $\text{HNO}_3$  bands. In order that a consistent set of profiles of  $\text{HNO}_3$  could be derived, the  $\nu_2$  band strength was scaled by 1.1. This awaits confirmation by experimental measurements, but it is still within the estimated absolute uncertainty of the band strengths and hence remains a valid choice.

#### IIF (14)

The line positions of the 1 - 0 fundamental were multiplied by a scaling factor of 0.99999989 to norm alize the original frequency calibration [61] to the current calibration standards for CO[62]. The resulting positions agree to better than  $0.00001 \text{ cm}^{-1}$  with the five heterodyne HF frequencies given by Goddon et al. [63]

#### HCl (15)

The computation error in the positions of all HCl lines on the 1992 HITRAN [6,64] were corrected using the work of Rinsland et al. [65] for the 1 - 0 band and all other bands from Tipping [66]. The intensities and widths were not changed and remain consistent with the measurements of Pine et al. [67,68]. The reference codes are 2 1 1 for the 1 - 0 band and 111 for the remainder.

#### ClO (18)

The updated parameters of the ClO fundamental near  $840 \text{ cm}^{-1}$  are taken from the work of Goldman et al. [69]. For these, the line positions have been calculated using the rotational constants of Burkholder et al. [70] with corrections of the presented Hamiltonian. Line intensities were computed according to the method outlined by Gillis and Goldman [71] using the dipole moment and Herman-Wallis terms reported by Burkholder et al. [72]. The averaged value of the N<sub>z</sub>-broadening coefficient of  $0.093 \text{ cm}^{-1}/\text{atm}$  at 296 K [72,73] is used for

the air-broadened widths and the temperature dependence coefficient is set 100.75 [73]. Additional details are given by Goldman et al. [69].

### OCS (19)

The carbonyl sulfide parameters were modified completely using newer results. The 1987 ATMOS linelists contained four infrared bands on the main list (from the 1982 AFGL tape) and two bands based on unpublished data in the supplemental linelist. The 1991 GEISA [7] provided a complete calculation of 19 infrared bands of the main isotope using positions obtained by Fayt and colleagues [74] and band strengths based on unpublished data and reported band strengths of Kagann [75 and the references therein]. Later, it was noticed that a computational error had occurred for the intensities, and a corrected prediction was kindly supplied by Fayt [76]. In addition, two isotopic bands of  $\nu_3$  based on the work of Blanquet et al. [77] were taken from the 1987 ATMOS linelist. The very old microwave prediction was removed. For air-broadened widths, the values on the 1992 HITRAN were assumed. For the self-broadened line widths, the measurements of Bouanich et al. [78] were merged. The temperature dependence coefficient measured for self-broadening [78] was employed for the air-broadening.

The update of the OCS parameters was much needed. There were sufficient experimental intensities that demonstrated that the  $\nu_3$  band strength needed to be increased on the compilations by almost 9%. Atmospheric investigators should note this difference when comparing present and prior OCS field measurements. However, the OCS linelist is incomplete because many isotopic and hot bands [79,62] have not been included.

### HOCl (21)

The HOCl parameters appearing in the 1992 HITRAN had not been updated since 1982, so the predictions of the  $\nu_2$  and  $\nu_3$  bands provided by Lafferty and Olson [80] for the 1987 ATMOS list was used. The  $\nu_1$  band has not been revised.

110, (22)

The approximate predictions of  $H_0$  in the 1987 supplemental list were replaced by predictions provided by Nelson and Zahniser [81-84] for all three fundamentals.

### **HO<sub>2</sub>NO<sub>2</sub>** (25)

The pseudolines from the supplemental linelist were removed so that the cross sections of May and Friedl [19] could be used instead.

### **ClONO<sub>2</sub>** (27)

The ClONO<sub>2</sub> parameters in the supplemental list have been described previously by Rinsland et al. [85] and are summarized here as a convenience to the reader. Near 780 cm<sup>-1</sup>, the experimental cross sections of Ballard et al. [86] have been set aside in favor of a line-by-line prediction based on the study by Bell et al. [87] of  $\nu_4$  of both isotopes of Cl and one hot band  $\nu_4 + \nu_9 - \nu_4$ . The relative intensities have been normalized to values of Ballard et al. [86], Davidson et al. [88] and Tuazon et al. [89], and results from other laboratory data [90]. The air-broadened coefficient was set to the averaged N<sub>2</sub>-width reported by Bell et al. with the temperature coefficient of 0.75 assumed. Parameters of the 1292 cm<sup>-1</sup> band published by Orphal et al. [90] are being sought along with revised predictions for the 780 cm<sup>-1</sup> band by McPheat and Duxbury [91].

### **CH<sub>3</sub>Cl** (30)

A prediction of the  $\nu_3$  region at 732 cm<sup>-1</sup> based on the positions of [92] and the intensities of Dang-Nhu et al. [93] has been added to the existing HITRAN parameters in the main list. In addition, a preliminary calculation of  $RQ_0$  at 1459 cm<sup>-1</sup> appears in the supplemental linelist. This has been obtained from a refinement of the Henfrey and Thrush study [94] by Tarrago et al. [95]. The linewidths of Blanquet et al. [96-98] have not been included, however, and no changes have been made to revise the incomplete prediction available for the 3.3  $\mu\text{m}$  region,

### **C F<sub>4</sub>(31)**

The 1987 parameters [3] for this species were a combination of a modified calculation of the Q branch of the  $\nu_3$  fundamental based on the work of Takami et al. [99] with measured P and R branch manifolds using the Fourier transform spectrometer at Kitt Peak. Since this list is incomplete, it is thought that it will soon be replaced either by cross sections [10, 23] or results of new analyses [100, 101]. The information given in Table 7 corresponds to the data of McDaniel et al. [10].

### **CCl<sub>2</sub>F<sub>2</sub> (32)**

The 922 cm<sup>-1</sup> band is represented by the cross sections of Varanasi and Nemtchinov [15,16]. All older pseudo-parameters (which contained only default values for the lower state energies) have been removed from the supplemental list. Figure 1 shows observed and synthetic spectra based on the new parameters.

### **CCl<sub>3</sub>F (33)**

The cross sections of Li and Varanasi [14] are being used for the CFC-11 bands, and so all data for this species has been removed from the supplemental list.

### **ccl, (35)**

The pseudolines in the 1987 supplemental list for this species has been removed from the supplemental list, and the cross sections of Orlando et al. [13] are being used. It should be noted that the new integrated intensity is 33% different from the value used for the 1987 linelist [3,9].

### **COClF (37)**

An experimental list of line positions in the  $\nu_1$  region near 1800 cm<sup>-1</sup> was obtained for the supplemental linelist using laboratory spectra recorded at Kitt Peak by one of the authors (Brown). The relative intensities are very crude line intensities (within a factor of 3). If this species were detected, much additional work would be needed to obtain adequate line parameters.

## **C<sub>2</sub>H<sub>6</sub>** (38)

In the 1987 ATMOS paper, we noted that there was a difference in reported intensity measurements for the  $\nu_9$  band near 820 cm<sup>-1</sup>. Daunt et al. [102] had produced a prediction whose integrated strength differed by 25% from that reported by Henry et al. [103] and an integrated RQ<sub>0</sub> strength of Goldman et al. [104]. The 1992 HITRAN contained the Daunt et al. prediction, but for the ATMOS linelist, we have normalized the intensities to match the other two studies.

The 1992 HITRAN included a representation of the Q branches of  $\nu_7$  near 3000 cm<sup>-1</sup> produced by Dang-Nhu and Goldman [105]. The 1987 ATMOS linelist contained a set of pseudolines obtained from unpublished Kitt Peak spectra and normalized to the intensities of Rinsland et al. [106]. Since the newer prediction was in poor agreement with the lab data, these parameters were removed from the main list. In the supplemental list, newer PQ<sub>3</sub> branch parameters from Rinsland et al. [107] were merged with approximate values from the 1987 supplemental list. The 3.3 μm region of ethane is very difficult to model [108] and thus still remains incompletely catalogued in all the databases. The only anticipated revisions for this region are the new intensity and air-broadening measurements of Pine et al. [109] for RQ<sub>0</sub> and PQ<sub>3</sub>.

## **C<sub>2</sub>H<sub>2</sub>** (40)

Two bands of C<sub>2</sub>H<sub>2</sub> at 3 μm were replaced using the positions and intensities of Auwera et al. [110] and the line widths of Devi et al. [111]. The other recent studies [112,113] have not yet been incorporated.

## **ClIF<sub>2</sub>Cl** (42)

The cross sections [10,17] are being used for the CFC-22 band, and so all older values for this species has been removed from the supplemental list. Newer cross sections [18] will eventually be used in place of the older values [10].

## **COCl<sub>2</sub>** (43)

Predictions of the ν<sub>1</sub> and ν<sub>5</sub> bands of phosgene based on the work of Yamamoto et al. [114] replaced

the approximate 1987 supplemental linelist parameters for this species. Default line widths of  $0.1 \text{ cm}^{-1}/\text{atm}$  were selected. If this species is ever detected, the assumed intensities will need to be validated.

#### HDO (49)

In the main list, nine bands of HDO parameters were labelled as molecule number 49 and isotope 1. In addition, a linelist of the V<sub>2</sub> band of HD<sup>18</sup>O from Toth via the 1987 ATMOS linelist [3] was added.

#### SF, (50)

The partial prediction of the v<sub>3</sub> region that appeared in the 1992 HITRAN database was removed so that the cross section data of Varanasi et al. [18] could be used. This change represents a significant improvement for the tropospheric retrievals.

### Database / Improvements Needed

Any atmospheric remote sensing investigation depends on the molecular database being complete and accurate. However, the databases generally have numerous faults and limitations because either existing laboratory data have not been included or sufficient laboratory studies have not been performed. At present, the molecular databases contain fairly reliable rotation-vibration line parameters or laboratory cross sections for many of the species for the far to mid-infrared spectral regions below 2800 cm<sup>-1</sup>. However, there are gaps for the near-infrared parameters, and no readily-available and well-documented public database exists for the visible and ultra-violet(Vis-UV) wavelengths. For example, some important deficiencies above 2800 cm<sup>-1</sup> include the omission of weak transitions of CH<sub>4</sub>, O<sub>3</sub>, H<sub>2</sub>O and N<sub>2</sub>O and a number of trace species. In addition, spectral effects occur in tropospheric data which are generally avoided in the lower pressure stratospheric regimes. The databases do not contain parameters to describe all the (high) pressure-induced phenomena that are required to compute tropospheric spectra. Some of these involving collision-induced continua can be obtained from individual sources, but insufficient studies have been done for the effects of line mixing in species like H<sub>2</sub>O and CH<sub>4</sub>.

The 1995 ATMOS and the 1995 HITRAN databases will not be exactly the same because the ATMOS catalog is tailored to meet the goals of a specific experiment operating in a designated spectral interval. The compilations will also differ because modification of the main ATMOS linelist was suspended in mid-1994 to facilitate a consistent basis for analysis of all ATMOS Shuttle data sets with the same molecular parameters. It is anticipated [115] that the 1995 HITRAN database will contain additional improvements. **Table 11** shows some of the changes that will be considered for revision of the ATMOS linelists.

At present, parameters in some form exist for all the detectable species that are being monitored by the ATMOS experiment. The database inaccuracies which affect retrievals the most are those associated with intensities since these propagate into the error budget of a retrieval on a 1:1 basis. To provide an overview of how spectroscopic uncertainties impact the retrievals, estimates of intensity uncertainties are given in Table 12 by species. The spectral regions used for ATMOS retrievals are shown to emphasize that these estimates pertain to only the parameters within the specific wavenumber intervals used by ATMOS and are not necessarily correct for all the intensities of a species throughout the database.. For example, the CH<sub>3</sub>D listed in Table 12 with 20% accuracies correspond only to the current parameters at 3.3  $\mu\text{m}$  (which has not been studied extensively in the laboratory); the CH<sub>3</sub>D parameters of the three revised fundamentals near 8  $\mu\text{m}$  (which are not being used for ATMOS retrievals) have accuracies closer to 7% [41]. The best accuracies of 3% are associated with linear species (CO, N<sub>2</sub>, HF, HCl, CO<sub>2</sub> and N<sub>2</sub>O) because the transitions of these fairly stable species are readily measured and modelled by simple expressions. The largest uncertainties of 15% to 20% occur for the heavier or less stable gases (HNO<sub>3</sub>, N<sub>2</sub>O<sub>5</sub>, ClONO<sub>2</sub>, and CCl<sub>4</sub>). The remainder fall in the range of 5- 10% depending on the species. These estimates in **Table 12** are thought to be conservative (perhaps 20) in that the numbers are generally larger than the values given in the original laboratory studies.

There are a number of laboratory studies that would significantly enhance the accuracy of the ATMOS retrievals. The absolute intensities of normal and <sup>18</sup>O substituted heavy ozone, are in need of improvement. As discussed previously, the 5% scaling of <sup>16</sup>O<sub>3</sub> intensities at 10  $\mu\text{m}$  based on the work of Pickett et al. [34] has not been adopted here since we believe further studies are needed to validate this result. Studies of heavy ozone enrichments require more accurate absolute intensities of <sup>16</sup>O<sup>16</sup>O<sup>18</sup>O and <sup>16</sup>O<sup>18</sup>O<sup>16</sup>O relative to <sup>16</sup>O<sub>3</sub>. This is a

difficult experimental problem given the fractionation effects known to occur in an electric discharge [116]. The 3000  $\text{cm}^{-1}$  region of  $\text{CH}_3\text{D}$  has never been successfully modelled to provide a prediction of relative intensities, and only a few individual line intensities have been measured [42]. Further studies are also needed to provide accurate intensities in nitric acid and carbon tetrachloride bands. Measurements and analyses of the numerous hot bands are needed for several molecules, especially those in the  $\nu_4$  region of  $\text{ClONO}_2$ , the  $\nu_3$  region of  $\text{SF}_6$  and all regions of the infrared bands of  $\text{HNO}_3$ . Absorption cross sections as a function of temperature and pressure are needed at 802  $\text{cm}^{-1}$  to improve retrievals of  $\text{HO}_2\text{NO}_2$ . Complete parameters for  $\text{C}_2\text{H}_6$  near 3000  $\text{cm}^{-1}$ , the  $\text{CH}_3\text{Cl}$  near 1400 and 3000  $\text{cm}^{-1}$ , and the isotopic OCS bands for the 500 to 4100  $\text{cm}^{-1}$  region are also needed, as well as general revision of the positions, intensities and widths of  $\text{H}_2\text{O}$  in the 600-1100  $\text{cm}^{-1}$  region of  $\text{H}_2\text{O}$ . It should be noted that these are the areas of highest priority for ATMOS and that additional problems exist in the databases which will seriously impact other remote sensing experiments.

## Conclusion

This article describes the 1995 ATMOS database of parameters used for the analysis of the atmospheric data recorded during the ATLAS 1,2 and 3 shuttle missions between 1992- and 1994. The updates have been done for the mid-infrared parameters of 26 gases. Anyone wishing to obtain these linclists should contact the first author.

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TABLE 1 SUMMARY OF THE ATMOS MAIN AND SUPPLEMENTAL MOLECULAR PARAMETERS

mol#	MOLECULE	#LINES	FMIN cm <sup>-1</sup>	FMAX cm <sup>-1</sup>	#ISO	#VIB	#BANDS	Total Intensity cm <sup>-1</sup> /molec. <sup>-1</sup> cm <sup>-2</sup> 296K	Sum
1	H <sub>2</sub> O	31016	0.40	9999.49	3	45	73	7.279 x10 <sup>-17</sup>	
2	CO <sub>2</sub>	60790	442.00	9648.00	8	319	589	1.126 x10 <sup>-16</sup>	
3	O <sub>3</sub>	196415	0.02	4060.78	5	92	104	1.836 x10 <sup>-17</sup>	
4	N <sub>2</sub> O	26249	0.83	5131.24	5	113	162	7.196 x10 <sup>-17</sup>	
5	CO	3600	3.46	8464.88	5	9	41	1.059 X10 <sup>-17</sup>	
6	CH <sub>4</sub>	45456	0.01	6184.49	3	40	51	1.772 x10 <sup>-17</sup>	
7	O <sub>2</sub>	1619	0.00	9468.43	3	6	9	9.107 x10 <sup>-24</sup>	
S 7	O <sub>2</sub>	162	1432.50	1676.96	1	1	1	1.470 X10 <sup>-27</sup>	
8	NO	7385	0.00	3966.00	3	42	50	4.730 x10 <sup>-18</sup>	
9	SO <sub>2</sub>	26225	0.01	2526.03	2	6	7	4.122 X10 <sup>-17</sup>	
10	NO <sub>2</sub>	44975	0.49	2938.37	1	9	9	6.241 x10 <sup>-17</sup>	
11	NH <sub>3</sub>	5817	0.21	2153.76	2	14	16	4.457 X10 <sup>-17</sup>	
12	HNO <sub>3</sub>	129741	0.03	1769.98	1	11	11	1.204 x10 <sup>-16</sup>	
s 12	HNO <sub>3</sub>	8751	845.11	908.83	1	2	2	3.246 x10 <sup>-18</sup>	
13	OH	3168	0.00	9997.35	3	39	43	4.554 X10 <sup>-17</sup>	
14	HF	84	41.11	7994.58	1	5	5	7.326 x10 <sup>-17</sup>	
15	HCl	324	20.24	8454.45	2	7	14	1.709 x10 <sup>-17</sup>	
16	HBr	398	16.23	9758.56	2	8	16	6.187 x10 <sup>-18</sup>	
17	HI	237	12.50	8487.30	1	9	9	1.096 x10 <sup>-18</sup>	
18	C1O	6038	0.01	886.21	2	4	8	1.160 x10 <sup>-18</sup>	
19	Ocs	4096	493.26	4117.99	3	19	21	1.068 x10 <sup>-16</sup>	
20	H <sub>2</sub> C O	2702	0.00	2998.52	3	8	10	2.326 x10 <sup>-17</sup>	
s 20	H <sub>2</sub> CO	587	1707.09	1781.38	1	1	1	7.195 x10 <sup>-18</sup>	
21	HOCL	15371	0.02	3799.68	2	4	8	3.235 x10 <sup>-17</sup>	
s 22	HO <sub>2</sub>	6820	1032.06	3675.81	1	4	4	1.795 X10 <sup>-17</sup>	
23	H <sub>2</sub> O <sub>2</sub>	5444	0.15	1499.48	1	2	2	1.872 x10 <sup>-17</sup>	
s 24	HONO	2348	779.12	1711.70	1	1	1	2.059 X10 <sup>-17</sup>	
c 25	HO <sub>2</sub> NO <sub>2</sub>		802.	804. (at 220K)				1.66 X10 <sup>-17</sup>	
c 26	N <sub>2</sub> O <sub>5</sub>		1210.	1275.				4.21 X10 <sup>-17</sup>	
s 27	ClONO <sub>2</sub>	23264	763.64	1309.99	2	3	4	3.113 X10 <sup>-17</sup>	
28	HCN	772	2.87	3421.96	3	6	8	3.086 X10 <sup>-19</sup>	
s 29	CH <sub>3</sub> F	739	987.91	1089.13	1	1	1	1.806 X10 <sup>-17</sup>	
30	CH <sub>3</sub> Cl	10432	661.79	3172.92	2	4	8	5.783 x10 <sup>-18</sup>	
s 30	CH <sub>3</sub> Cl	621	1324.69	1460.14	2	2	3	1.163 x10 <sup>-18</sup>	
c 31	CF <sub>4</sub>		1255.0	1289.				1.61 x10 <sup>-16</sup>	
c 32	CCl <sub>2</sub> F <sub>2</sub>		810.	965.				5.95 X10 <sup>-17</sup>	
c 33	CCl <sub>3</sub> F		810.	880.				6.95 x10 <sup>-17</sup>	
s 34	CH <sub>3</sub> CCl <sub>3</sub>	251	1382.50	1385.00	1	1	1	1.25 x10 <sup>-19</sup>	
c 35	CCl <sub>4</sub>		770.00	809.99				5.14 X10 <sup>-17</sup>	
36	COF <sub>2</sub>	33932	725.00	1981.27	1	7	7	1.195 x10 <sup>-16</sup>	
s 37	CFC1O	2449	764.11	1907.92	1	2	2	3.957 X10 <sup>-17</sup>	
38	C <sub>2</sub> H <sub>6</sub>	10000	745.22	951.65	1	1	1	6.967 x10 <sup>-19</sup>	
s 38	C <sub>2</sub> H <sub>6</sub>	115	2976.63	2996.98	1	1	1	2.875 x10 <sup>-18</sup>	
40	C <sub>2</sub> H <sub>2</sub>	1267	638.25	3374.22	2	8	9	4.103 X10 <sup>-17</sup>	
41	N <sub>2</sub>	120	1992.62	2625.40	1	1	1	6.719 x10 <sup>-27</sup>	
C 42	CHF <sub>2</sub> Cl (FTS)		780.	839.				2.05 X10 <sup>-17</sup>	
c 42	CHF <sub>2</sub> Cl (TDL)		828.95	829.16				3.11 x10 <sup>-19</sup>	
s 43	Coc 1 <sub>2</sub>	32871	828.54	1862.45	1	2	2	3.35 X10 <sup>-19</sup>	
s 44	CH <sub>3</sub> Br	3421	871.32	1038.06	1	1	1	6.427 x10 <sup>-19</sup>	
s 45	CH <sub>3</sub> I	2528	793.46	971.65	1	1	1	1.207 x10 <sup>-18</sup>	
s 46	HCOOH	3388	1060.96	1161.25	1	1	1	1.757 x10 <sup>-17</sup>	
47	H <sub>2</sub> S	661	994.12	1573.81	1	1	1	7.959 x10 <sup>-20</sup>	
s 48	CHFCl <sub>2</sub>	9583	785.00	1099.99	1	1	1	5.284 x10 <sup>-17</sup>	
49	HDO	8505	0.01	5507.54	2	9	10	7.694 x10 <sup>-21</sup>	
c 50	SF <sub>6</sub>		940.42	952.23				5.243 x10 <sup>-17</sup>	

The ATMOS Main list 694359 lines from o to 9999 cm<sup>-1</sup>  
The ATMOS Supplemental list s : 116016 lines from 725 to 3675 cm<sup>-1</sup>  
The ATMOS Cross Section list c : 8 species from 77(l) to 1289 cm<sup>-1</sup>

**Table 2** Sample of the 1995 ATMOS main and supplemental linelists

Molecule	#	1s0	Position	Intensity	E	Air-y	Self-y	r2	n	Shift	V <sub>1P</sub>	V <sub>1O</sub>	Rotational	acc	refs	
O3	3	1	971.210600	5.010E-25	2497.4550	.0691	.0849	1.678E-02	0.760.000000	19	8231311		241312	005	111	
C02	2	4	971.214903	7.000E-27	1410.1167	.0790	.1091	7.013E-04	0.700.000000	9	5	R	9	425	111	
O3	3	2	971.221900	1.000E-24	1216.2510	.0650	.0890	1.612E-02	0.760.000000	5	1	52548	53549	002	112	
COF2	36	1	971.229400	1.361E-21	50.1023	.0845	.1750	0.000E+00	0.940.000000	10	1	1294	1193	0000	111	
CH3Br	44	1	971.229500	2.040E-22	377.1063	.1000	.0000	0.000E+00	0.75	0.000000	27	1433	3	33	2	
COF2	36	1	971.229600	1.360E-21	50.1021	.0845	.1750	0.000E+00	0.940.000000	10	1	1284	1183	0000	111	
O3	3	2	971.230400	8.240E-25	1245.7990	.0651	.0890	1.562E-02	0.760.000000	5	1	51	744	52	745	
O3	3	1	971.231000	4.470E-25	472.7870	.0708	.0914	7.651	E-070.76	0.000000	5	1	26621	25	818	
CH3I	45	1	971.235400	6.000E-23	854.2444	.1000	.0000	0.000E+00	0.75	0.000000	27	1447	9	46	8	
O3	3	3	971.235500	1.010E-23	667.9365	.0692	.0905	1.669E-02	0.760.000000	5	1	34	728	35	729	
CH3Br	44	1	971.239900	9.350E-23	404.9513	.1000	.0000	0.000E+00	0.75	0.000000	27	14	36	0	35	1

Positions are in cm<sup>-1</sup>. Intensities are in cm<sup>-1</sup>/(molecule·cm<sup>2</sup>) at 296 K. Line widths and shifts are in cm<sup>-1</sup>/atm at 296 K.

TABLE 3 SUMMARY OF ISOTOPES CODES AND ABUNDANCES

MOL NUM	SPECIES	ISO NUM	OLD CODE	FORMULA	ABUNDANCE	MOL NUM	SPECIES	ISO NUM	OLD CODE	FORMULA	ABUNDANCE
1	$\text{H}_2\text{O}$	1	161	$\text{H}_2^{16}\text{O}$	0.9373	18	$\text{ClO}$	1	50	$^{35}\text{Cl}^{16}\text{O}$	0.7559
		2	181	$\text{H}_2^{18}\text{O}$	0.002000			2	78	$^{37}\text{Cl}^{16}\text{O}$	0.2417
		3	171	$\text{H}_2^{17}\text{O}$	0.000372			19	822	$^{16}\text{O}^{12}\text{C}^{32}\text{S}$	0.8374
2	$\text{CO}_2$	1	828	$^{12}\text{C}^{16}\text{O}^{16}\text{O}$	0.8842	20	$\text{H}_2\text{CO}$	2	624	$^{16}\text{O}^{12}\text{C}^{34}\text{S}$	0.04158
		2	838	$^{13}\text{C}^{16}\text{O}^{16}\text{O}$	0.01108			3	632	$^{16}\text{O}^{13}\text{C}^{32}\text{S}$	0.01053
		3	828	$^{12}\text{C}^{16}\text{O}^{18}\text{O}$	0.003947			4	822	$^{18}\text{O}^{12}\text{C}^{32}\text{S}$	0.001880
		4	827	$^{12}\text{C}^{16}\text{O}^{17}\text{O}$	0.000734			1	128	$\text{H}^{12}\text{C}^{16}\text{O}$	0.9882
		5	83s	$^{13}\text{C}^{16}\text{O}^{18}\text{O}$	0.00004434			2	138	$\text{H}^{2}\text{C}^{13}\text{O}$	0.01108
		6	837	$^{13}\text{C}^{16}\text{O}^{17}\text{O}$	0.00000825			3	128	$\text{H}^{2}\text{C}^{18}\text{O}$	0.00
		7	828	$^{12}\text{C}^{18}\text{O}^{16}\text{O}$	0.000003957			21	165	$\text{H}^{16}\text{O}^{35}\text{Cl}$	0.755s
		8	728	$^{12}\text{C}^{17}\text{O}^{18}\text{O}$	0.00000147			2	187	$\text{H}^{16}\text{O}^{37}\text{Cl}$	0.2417
3	$\text{O}_3$	1	666	$^{16}_0\text{O}^{16}_0\text{O}^{16}_0$	0.9929	22	$\text{HO}_2$	1		$\text{HO}_2$	1.0
		2	88s	$^{16}_0\text{O}^{16}_0\text{O}^{18}_0$	0.003982			23	1881	$\text{H}_2\text{O}_2$	0.9950
		3	666	$^{16}_0\text{O}^{18}_0\text{O}^{16}_0$	0.001991			24		$\text{HNO}_2$	1.0
		4	687	$^{16}_0\text{O}^{16}_0\text{O}^{17}_0$	0.000744			25		$\text{HN}_0$	1.0
		5	678	$^{16}_0\text{O}^{17}_0\text{O}^{16}_0$	0.000372			26		$\text{N}_2\text{O}_3$	1.0
4	$\text{N}_2\text{O}$	1	448	$^{14}_N^{14}_N^{16}\text{O}$	0.9903	27	$\text{ClONO}_2$			$\text{ClONO}_2$	1.0
		2	458	$^{14}_N^{15}_N^{16}\text{O}$	0.003641			28	124	$^{12}\text{C}^{14}_N$	0.9851
		3	546	$^{15}_N^{14}_N^{16}\text{O}$	0.003641			2	134	$^{13}\text{C}^{14}_N$	0.01107
		4	448	$^{14}_N^{14}_N^{18}\text{O}$	0.001988			3	125	$^{12}\text{C}^{15}\text{N}$	0.003622
		5	447	$^{14}_N^{14}_N^{17}\text{O}$	0.000369			29		$\text{CH}_3\text{F}$	1.0
5	$\text{CO}$	1	20	$^{12}\text{C}^{16}\text{O}$	0.885	30	$\text{CH}_3\text{Cl}$	1	215	$^{12}\text{CH}_3^{35}\text{Cl}$	0.7489
		2	38	$^{13}\text{C}^{16}\text{O}$	0.01108			2	217	$^{12}\text{CH}_3^{37}\text{Cl}$	0.2385
		3	28	$^{12}\text{C}^{18}\text{O}$	0.301078			31		$\text{CF}_4$	1.0
		4	27	$^{12}\text{C}^{17}\text{O}$	0.000388			32		$\text{CCl}_2\text{F}_2$	1.0
		5	3s	$^{13}\text{C}^{18}\text{O}$	0.00002222			33		$\text{CCl}_3\text{F}$	1.0
6	$\text{CH}_4$	1	211	$^{12}\text{CH}_4$	0.8883	34	$\text{CH}_3\text{OCl}_3$	1		$\text{CH}_3\text{CCl}_3$	1.0
		2	311	$^{13}\text{CH}_4$	0.01110			35		$\text{CCl}_4$	1.0
		3	212	$^{12}\text{CH}_3\text{D}$	0.0006158			38		$\text{COF}_2$	0.9885
7	$\text{O}_2$	1	66	$^{16}_0\text{O}^{16}_0$	0.0953	37	$\text{OCOCF}_3$	1		$\text{CO}_\text{W}$	1.0
		2	68	$^{16}_0\text{O}^{18}_0$	0.003981			38	1221	$\text{C}_2\text{H}_6$	0.9770
		3	67	$^{16}_0\text{O}^{17}_0$	0.000742			39		$\text{C}_2\text{H}_4$	1.0
8	$\text{NO}$	1	48	$^{14}_N^{16}\text{O}$	0.8949	40	$\text{C}_2\text{H}_2$	1	1221	$^{12}\text{O}^{12}\text{CH}_2$	0.0776
		2	58	$^{15}_N^{16}\text{O}$	0.003654			2	1231	$^{12}\text{C}^{13}\text{CH}_2$	0.02107
		3	4s	$^{14}_N^{18}\text{O}$	0.001993			41	44	$\text{N}_2$	0.927
9	$\text{SO}_2$	1	626	$^{32}\text{S}\text{O}_2$	0.9457	42	$\text{CHF}_2\text{Cl}$	1		$\text{CHF}_2\text{Cl}$	1.0
		2	848	$^{34}\text{S}\text{O}_2$	0.04195			43		$\text{COCl}_2$	1.0
10	$\text{NO}_2$	1	848	$\text{NO}_2$	0.8916	44	$\text{CH}_3\text{Br}$	1		$\text{CH}_3\text{Br}$	1.0
		11	4111	$^{14}\text{N}\text{H}_3$	0.9959			45		$\text{CH}_3\text{I}$	1.0
12	$\text{HNO}_3$	1	5111	$^{15}\text{NH}_3$	0.003881	48	$\text{HOOOH}$	1		$\text{HCOOH}$	1.0
		2	148	$\text{HNO}_3$	0.8891			47		$\text{H}_2\text{S}$	0.8499
		13	61	$^{16}\text{OH}$	0.9975			2		$\text{H}_2^{34}\text{S}$	0.049
		2	81	$^{18}\text{OH}$	0.002000			3		$\text{H}_2^{33}\text{S}$	0.001
14	$\text{HF}$	1	19	$\text{HF}$	0.0998	48	$\text{CHFCl}_2$	1		$\text{CHFCl}_2$	1.0
		15	15	$\text{H}^{35}\text{Cl}$	0.7576			2			
16	$\text{HBr}$	2	17	$\text{H}^{37}\text{Br}$	0.2423	49	$\text{HDO}$	1	182	$\text{HD}^{16}\text{O}$	0.0003107
		1	19	$\text{H}^{79}\text{Br}$	0.5088			2	182	$\text{HD}^{18}\text{O}$	0.0000006
17	$\text{HI}$	1	17	$\text{HI}$	0.9998	50	$\text{SF}_6$	1		$^{32}\text{SF}_6$	0.9502

TABLE 4 VIBRATIONAL QUANTUM NUMBERS CORRESPONDING TO LINELIST INDEX CODE  $V_{UP}$  and  $V_{LO}$

Group 1 : $H_2O$ , $O_3$ , $S O_2$ , $NO_2$ , $HOCl$ , $HDO$ , $HO_2$ , $H_2S (v_1, v_2, v_3)$									
1) $O\bullet O$	2) 010	3) 020	4) 100	5) 001	6) 030	7) 110	8) 011		
9) 040	10) 120	11) 021	12) 200	13) 101	14) 002	15) 130	16) 031		
17) 210	18) 111	19) 012	20) 041	21) 220	22) 121	23) 022	24) 300		
25) 201	26) 102	27) 003	28) 131	29) 310	30) 211	31) 112	32) 013		
33) 141	34) 042	35) 320	36) 221	37) sol	38) 202	39) 122	40) 023		
41) 400	42) 103	43) 004	44) 151	45) 330	46) 231	47) 212	48) 311		
49) 410	50) 113	51) 321	52) 222	53) 302	54) 401	55) 420	56) 123		
57) 600	58) 203	59) 104	60) 61)	61) 331	62) 213	63) 312	64) 411		
65) S03	66) 402	67) 403	68) 421	69) 501	70) 313	71) 412	72) 232		
73) 050	74) Oeo								
Group 2 : $CO_2$ ( $v_1, v_2, l_2, v_3$ , index)									
1) 00001	2) 01101	3) 10202	4) 02201	5) 10001	6) 11102	7) 03301	8) 11101		
9) 00011	10) 20003	11) 12202	12) 20002	13) 04401	14) 12201	15) 20001	16) 01111		
17) 21103	18) 13302	19) 21102	20) 05501	21) 13301	22) 21101	23) 10012	24) 02211		
25) 10011	28) 30004	27) 22203	28) 14402	29) 30003	30) 22202	31) 06601	32) 30002		
33) 14401	34) 22201	35) 30001	36) 11112	37) 03311	38) 11111	39) 00021	40) 31104		
41) 31103	42) 31102	43) 20013	44) 12212	45) 23301	46) 31101	47) 04411	48) 20012		
49) 12211	50) 20011	51) 01121	52) 40004	53) 32203	54) 21113	55) 40002	56) 13312		
57) 05511	56) 21112	59) 13311	60) 21111	61) 10022	62) 02221	63) 10021	64) 30014		
65) 22213	66) 14412	67) 41102	es) 30313	69) 06611	70) 22212	71) 30012	72) 41101		
73) 14411	74) 22211	75) 30011	76) 11122	77) 03321	78) 11121	79) 00031	so) 31114		
81) 23313	82) 31113	83) 23312	84) 31112	85) 15511	86) 20023	87) 23311	as) 12222		
68) 31111	69) 20022	91) 12221	92) 20021	93) 01131	94) 40015	95) 32214	96) 40014		
97) 32213	98) 40013	89) 51102	100) 32212	101) 40012	102) 21123	103) 32211	104) 21122		
105) 40011	106) 21121	107) 10032	108) 02231	109) 10031	110) 41114	111) 41113	112) 41112		
113) 11132	114) 03331	115) 11131	116) 20033	117) 12232	118) 20032	119) 12731	120) 20031		
121) 21133	122) 21132	123) 21131	124) 23303	125) 15502	126) 23302	127) 07701			
Group 3 : $N_2O$ , $OCS$ , $HCN$ ( $v_1, v_2, l_2, v_3$ )									
1) Oooo	2) 0110	3) 0200	4) 0220	5) 1000	6) 0310	7) 0330	8) 1110		
9) 0400	10) 0420	11) 1203	12) 1220	13) 2000	14) 0001	15) 0510	16) 1310		
17) 1s30	16) 2110	19) 0111	20) 14C0	21) 1420	22) 2200	23) 2220	24) 3000		
25) 0201	26) 0221	27) 1001	28) 2310	29) 3110	30) 0311	31) 0331	32) 1111		
33) 4000	34) 3200	35) 2001	se) 1201	37) 1221	38) 0032	39) 2111	40) 0112		
Group 4 : $CO$ , $HF$ , $HCl$ , $HBr$ , $HI$ , $N_2$									
1) o	2) 1	3) 2	4) 3	5) 4	6) 5				
Group 5 : $CH_4$ , $CF_4$ , $CCl_4$ , $HONO$ , $HCOOH$ , $SF_6$ , $CH_3D$ , $CH_3Cl$ , $CH_3Br$ , $CH_3I$ , $C$ , $H_3F$ , $C_2H_6$ , $HNO_3$ , $N_2O_5$ , $ClONO_2$ , $CCl_2F_2$ , $CCl_3F$ , $CHF_2Cl$ , $CHFCI_2$									
1) 00000000	2) 00000111	3) 01100001	4) 0000202	5) 00000222	6) 01100112				
7) 10000000	6) 03011001	9) 02200302	10) 10000111	11) 00011112	12) 01111002				
13) 00022002	14) GROUND	15) VI	16) V2	17) V4	18) V5				
1 e) V9	20) 2V5	21) 2V9	22) 3V6	23) 3V9	24) V5 + V9				
25)	26) V6	27) v 3	28) 2V6	29) 00000333	30) 00211223				
31) w	32) V6	33) V6 + V9							
Group 6 : $O_2$									
1) Xo	2) xl	3) Ao	4) A1	5) 60	6) El	7) B2			
Group 7 : $NO$ , $o H$ , $CIO$									
1) X3/2 0	2) X3/2 1	3) X3/2 2	4) X3/2 3	5) X3/2 4	6) X3/2 5	7) X3/2 6	8) X3/2 7		
9) X3/2 8	10) X3/2 9	11) xl/2 o	12) xl/2 1	13) X1/2 2	14) X1/2 3	15) xl/2 4	16) X1/2 5		
17) xl/2 6	18) X1/2 7	19) X1/2 8	20) xl/2 9						
Group 8 : $NH_3$ ( $v_1, v_2, v_3, v_4$ , inversion)									
1) Oooo	2) 0100	3) 0200	4) 0001	5) 0000A	6) 01 00A	7) 0200A			
8) 0001A	9) 0000S	10) 0100S	11) 0200s	12) 0001S					
Group 9 : $H_2CO$ , $H_2O_2$ , $COF_2$ , $COCl_2$ , $COClF$ ( $v_1, v_2, v_3, v_4, v_5, v_6$ )									
1) 000000	2) 000002	3) 001100	4) 031001	5) 100000	6) 000010	7) 010100	6) 010001		
9) 000001	10) 010000	11) 000100	12) 020000	13)	14) 002001	15) 000020			
Group 10: $C_2H_2$ ( $v_1, v_2, v_3, l_3, v_4, l_4, v_5, l_5$ )									
1) 000000000	2) 000001111	3) 001000000	4) 010111100	5) 0001 1001 6)					
7) IYY311110	8) 000111112	e) 00000200	10) 00000222						

Table 5 Definition of the Accuracy Codes

	Wavenumber		Intensity and Halfwidth
<u>ACC</u>	<u>Error Range</u>	<u>ACC</u>	<u>Error Range</u>
0	$\geq 1.$ or Undefined	0	Undefined
1	$\geq 0.1$ and $< 1.$	1	Default or Constant
2	$\geq 0.01$ and $< 0.1$	2	Average or Estimate
3	$\geq 0.001$ and $< 0.01$	3	$\geq 20\%$
4	$\geq 0.0001$ and $< 0.001$	4	$\geq 10\%$ and $< 20\%$
5	$\geq 0.00001$ and $< 0.0001$	5	$\geq 5^{\circ}\text{A}$ and $< 10^{\circ}\text{A}$
6	$< 0.00001$	6	$\geq 2^{\circ}\text{A}$ and $< 5^{\circ}\text{A}$
		7	$\geq 10/0$ and $< 27/0$
		8	$< 1\%$

Table 6 Molecule Numbers on the ATMOS (A), HITRAN (H) and GEISA (G) Databases

Species	A	H	G	Species	A	H	G	Species	A	H	G
H <sub>2</sub> O	1	1	1	ClO	18	18	19	CCl <sub>4</sub>	35	0	0
CO <sub>2</sub>	2	2	2	OCS	19	19	20	COF <sub>2</sub>	36	29	38
O <sub>3</sub>	3	3	3	H <sub>2</sub> CO	20	20	21	CFCIO	37	0	0
N <sub>2</sub> O	4	4	4	HOCl	21	21	32	C <sub>2</sub> H <sub>6</sub>	38	27	22
c O	5	5	5	HO <sub>2</sub>	22	0	0	C <sub>2</sub> H <sub>4</sub>	39	0	25
CH <sub>4</sub>	6	6	6	H <sub>2</sub> O <sub>2</sub>	23	25	35	C <sub>2</sub> H <sub>2</sub>	40	26	24
O <sub>2</sub>	7	7	7	HONO	24	0	0	N <sub>2</sub>	41	22	33
NO	8	8	8	HO <sub>2</sub> NO <sub>2</sub>	25	0	0	CHF <sub>2</sub> Cl	42	0	0
SO*	9	9	9	N <sub>2</sub> O <sub>5</sub>	26	0	0	COCl <sub>2</sub>	43	0	0
NO <sub>2</sub>	10	10	10	ClONO <sub>2</sub>	27	0	0	CH <sub>3</sub> Br	44	0	0
NH <sub>3</sub>	11	11	11	HCN	28	23	27	CH <sub>3</sub> I	45	0	0
HNO <sub>3</sub>	12	12	13	CH <sub>3</sub> F	2	9	0	HCOOH	46	32	37
OH	13	13	14	CH <sub>3</sub> Cl	30	24	34	H <sub>2</sub> S	47	31	36
HF	14	14	15	CF <sub>4</sub>	31	0	0	CHFCI <sub>2</sub>	48	0	0
HCl	15	15	16	CCl <sub>2</sub> F <sub>2</sub>	32	0	0	HDO	49	1	1
HBr	16	16	17	CCl <sub>3</sub> F	3	3	0	SF <sub>6</sub>	50	30	39
HI	17	17	18	CH <sub>3</sub> CCl <sub>3</sub>	34	0	0	CH <sub>3</sub> D	6	6	23

GEISA species GH<sub>4</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>2</sub>N<sub>2</sub>, C<sub>4</sub>H<sub>2</sub>, HC<sub>3</sub>N, C<sub>3</sub>H<sub>4</sub> AND PH<sub>3</sub> are excluded from the ATMOS lists.

**Table 7** Summary of Absorption Cross Sections used for ATMOS Retrievals

Molecule	Ref.	Spectral Range cm-1	Temp. K	Press, atm.	Integrated cm <sup>-1</sup> / (molecule cm <sup>-2</sup> )	Strength cm <sup>-1</sup> /pt	Grid cm <sup>-1</sup> /pt
<b>CCl<sub>2</sub>F<sub>2</sub></b>	15,16	<b>810.04 - 964.98</b>	<b>216</b>	<b>0.2236</b>	5.951>17	0.010	
		810.04- 964.93	233	<b>0.259s</b>	5.941s17		
		810.06- 964.93	245	<b>0.4675</b>	<b>5.931s-17</b>		
		810.05- 964.96	260	<b>0.8612</b>	<b>5.941s-17</b>		
		810.02- 964.98	273	<b>0.6509</b>	<b>5.901s-17</b>		
		<b>810.08- 964.97</b>	<b>284</b>	<b>0.6845</b>	<b>5.891s-17</b>		
		<b>810.01- 964.96</b>	<b>296</b>	<b>0.9214</b>	<b>5.951s-17</b>		
<b>CCl<sub>3</sub>F</b>	14	<b>810.01- 879.98</b>	<b>215</b>	<b>0.2242</b>	<b>6.881s-17</b>	0.012	
			225	<b>0.2278</b>	6.891>17		
			233	<b>0.3299</b>	<b>6.851s-17</b>		
			246	<b>0.3800</b>	6.861>17		
			272	<b>0.7242</b>	<b>6.921s-17</b>		
			284	<b>0.6857</b>	<b>6.951s-17</b>		
			296	<b>0.9991</b>	6.951s17		
<b>c1 HF<sub>2</sub>Cl</b> (FTS)	10	780.01- 840.00	203	N/A	1.881}>17	0.015	
			213		1.901s-17		
			233		1.941s-17		
			2.53		1.991517		
			273		2.011>17		
			293		<b>2.051s-17</b>		
			17				
(1'1)1.)	17	828.95- 829.16	216	0.0527	<b>4.471s-19</b>	0.00026	
		828.95- 829.16	216	<b>0.1017</b>	<b>4.491s-19</b>		
		828.95- 829.16	216	<b>0.1480</b>	<b>4.401s-19</b>		
		828.95- 829.16	216	<b>0.2369</b>	<b>4.271s-19</b>		
		828.94- 829.19	236	<b>0.3548</b>	<b>4.251s-19</b>		
		828.94- 829.19	252	<b>0.s288</b>	<b>3.791s-19</b>		
		828.94- 829.18	292	<b>0.9983</b>	<b>3.111s-19</b>		
<b>HNO<sub>2</sub>NO<sub>2</sub></b>	19	769.99- 834.99	220	N/A	1.721>17	0.00247	
<b>N<sub>2</sub>O<sub>5</sub></b>	11	1210.15-1275.76	233	N/A	<b>3.891s-17</b>	0.482	
			253		<b>4061s-17</b>		
			273		<b>4.091s-17</b>		
			293		<b>4.211s-17</b>		
<b>CCl<sub>4</sub></b>	13	770.01- 809.99	170	N/A	4.901s-17	0.0048	
			223		4.951s-17		
			<b>2 4 8</b>		5.071s-17		
			273		5.061s-17		
			298		5.101s-17		
			310		5.141s-17		
<b>CF<sub>4</sub></b>	10	<b>12.5s.01 -1289.99</b>	203	N/A	1.521s-16	0.015	
			213		1.651s-16		
			233		1.591s-16		
			253		<b>1.651s-16</b>		
			273		1.621s-16		
			293		1.611s-16		
<b>SF<sub>6</sub></b>	18	<b>92S.00 - 95S.00</b>	295	1.00	2.071s-16	0.010	
			273	0.723	2.051s-16		
			246	<b>0.468</b>	<b>2.091s-16</b>		
			216	<b>0.0329</b>	<b>2.551s-16</b>		

**Table 8 Differences between the 1995 ATMOS and 1992 HITRAN Databases**

SPECIES	REGION	v	I	y	REFERENCES
H <sub>2</sub> O	replace some 2v <sub>2</sub> lines at 3 μm replace some rotational lines 12 -8.7 μm		*	*	25 24
O <sub>3</sub>	10 μm, 3.3 μm, 2.7 μm, 2.5 μm, and 14 μm isotopes	*	*		29-33
N <sub>2</sub> O	3.3 μm to 3.0 μm bands	*	*	*	39,40
CH <sub>3</sub> D	v <sub>3</sub> , v <sub>5</sub> , v <sub>6</sub> triad at 7 μm -9 μm		*		41
O <sub>2</sub>	6 μm	*	*		44,45
NO	1 -0 (all) and all widths above 1600 cm <sup>-1</sup>	*	*	*	46
NO <sub>2</sub>	6 μm (v <sub>3</sub> , 2v <sub>2</sub> , v <sub>2</sub> +v <sub>3</sub> -v <sub>2</sub> ) bands	*	*	*	48-50
HNO <sub>3</sub>	v <sub>5</sub> , 2v <sub>9</sub> (11μ) v <sub>2</sub> , v <sub>3</sub> , v <sub>4</sub> regions intensities scaled	*	*		53,54 56-59
HF	1 -0 positions * 0.99999989.36 (f 13)	*			61,63
HCl	all bands	*			64-66
ClO	1 -0 near 12 μm	*	*		69-73
OCS	500-4100 cm <sup>-1</sup> for 21 bands	*	*	*	74-78
HOC]	v <sub>2</sub> , v <sub>3</sub> near 14 μm, 8.1 μm region	*			80
HO <sub>2</sub>	fundamentals 3-9 μm	*	*		81-84
C1ONO,	v <sub>4</sub> near 13 μm	*	*	*	85-89
c} I <sub>3</sub> Cl	v <sub>3</sub> near 15 μm v <sub>5</sub> RQ <sub>o</sub> branch only	*	*		92,93 94,95
COClF	approximate parameters for v <sub>1</sub> at 5.5 μm	*			PRESENT
C <sub>2</sub> H <sub>6</sub>	v <sub>9</sub> near 12 μm 19873 μm Q Branches + PQ <sub>3</sub>		*	*	102-103 104-107
C <sub>2</sub> H <sub>2</sub>	3 μm	*	*		110
COCl <sub>2</sub>	VI, v <sub>5</sub> bands near 5.5 μm and 11 μm	*	*		114
HD <sup>18</sup> O	V <sub>2</sub> near 7.2 μm	*	*		3

**Table 9 Summary of Alterations to the Main ATMOS Linelist**

SPECIES	1SO	#LINES	FMIN cm <sup>-1</sup>	FMAX cm <sup>-1</sup>	I MIN cm <sup>'''</sup>	1 MAX /(molecule x cm <sup>-2</sup> )	S-SUN	ACC	REF	PBHW	P MAX (cm <sup>-1</sup> /atm)	SELF_WAX	NTDP	NMAX (cm <sup>-1</sup> /atm)				
H <sub>2</sub> O	( 1)																	
000	000	1	1731	0.401	1647.767	1. 01E-32	2.67E-18	5.268E-17	000	0	0	0	0.0080.105	0.0000.000				
020	000	1	1132	2565.280	4338.475	1.00E-26	2.98E-21	8.161E-20	000	0	0	0	0.0090.105	0.0000.000				
O <sub>3</sub>	( 3)																	
010	000	4	5641	584.251	820.380	3.51E-27	5.57E-25	3.804E-22	450	5	5	0	0.065	0.0870.0790.1120.760.76				
010	000	5	2846	591.161	822.795	3.52E-27	6.06E-25	2.075E-22	450	5	5	0	0.065	0.0870.0790.1120.760.76				
102	101	1	1130	922.344	1002.238	9.94E-26	2.69E-24	8.293E-22	45044	0	0.065	0.0870.083	0.111	0.760.76				
003	101	1	192	931.056	1004.900	9.93E-26	6.38E-25	4.092E-23	45044	0	0.0670.0820.0880.101	0.760.76						
201	200	1	791	931.896	1008.602	9.92E-26	9.81E-25	2.941E-22	45044	0	0.0670.0870.0880.112	0.760.76						
003	002	1	1364	935.836	1020.250	9.90E-26	5.16E-24	1.666E-21	4504	4	0.065	0.0870.081	0.1120.760.76					
102	002	1	206	940.504	1014.917	9.95E-26	6.37E-25	4.723E-23	45044	0	0.0670.082	0.0870.0990.760.76						
300	101	1	196	1159.487	1208.161	9.98E-26	2.61.83E-25	2.671E-23	4504	4	0	0.071	0.084	0.0970.1090.760.76				
003	100	1	1270	1863.333	2093.154	1.00E-25	3.90E-24	1.234E-21	4504	4	0	0.065	0.0870.083	0.112	0.760.76			
102	100	1	1132	1885.468	2064.958	1.00E-25	2.31E-24	3.704E-22	4504	4	0	0.065	0.0860.081	0.111	0.760.76			
003	001	1	1861	1894.594	2088.217	1.00E-25	1.22E-23	1.507E-21	4504	4	0	0.065	0.0870.082	0.111	0.760.76			
102	001	1	2159	1966.935	2066.712	1.02E-25	4.32E-24	3.146E-20	45044	0	0.064	0.0870.0760.111	0.760.76					
201	100		1968	1999.192	2132.692	1.00E-25	3.00E-23	1.041E-20	450	4	4	0	0.064	0.0870.0780.112	0.76	0.76		
201	001		948	2014.848	2204.232	1.00E-25	1.91E-24	2.468E-22	45044	0	0	0.0660.0860.0800.110	0.760.76					
300	100		849	2101.905	2251.240	1.00E-25	2.172E-24	2.174E-22	4504	4	0	0.065	0.084	0.0860.110	0.760.76			
300	001		1075	2210.164	2302.772	1. 01E-25	2.73E-24	8.457E-22	4504	4	0	0.0660.0870.083	0.111	0.760.76				
103	100		970	2841.156	2930.506	1.00E-25	1.83E-24	5.530E-22	450	2	200.065	0.0870.085	0.1120.760.76					
103	001		200	2873.465	3019.922	1.00E-25	2.54E-24	1.040E-22	450	2	20	0.0660.084	0.0860.1080.760.76					
310	100		15	2877.462	2927.423	1. 01E-25	3.26E-25	2.731E-24	45022	0	0.071	0.0780.093	0.104	0.760.76				
004	100		125	2877.632	2972.559	1. 01E-25	7.59E-25	2.611E-23	45022	0	0.0690.084	0.0860.1060.760.76						
004	001		1452	2878.938	2992.258	1.00E-25	9.18E-24	2.941E-21	450	2	2	0	0.065	0.0870.081	0.111	0.760.76		
310	001	1	142	2882.411	2974.307	1. 01E-25	7.88E-25	2.670E-23	450	2	2	0	0.065	0.0770.0860.1040.760.76				
013	010	1	1639	2902.203	3049.761	1.00E-25	1.22E-23	4.026E-21	450	2	2	0	0.065	0.0870.080	0.112	0.76		
112	010	1	636	2923.918	3102.695	1.00E-25	1.76E-24	1.707E-22	45022	0	0.065	0.084	0.0880.1090.760.76					
003	000	1	3394	2926.875	3192.978	1.00E-25	4.05E-25	2.1306E-19	4504	4	0	0.064	0.0870.0720.1120.760.76					
102	000	1	3103	2938.639	3175.149	1.00E-25	6.65E-23	1.231E-20	4504	4	0	0.064	0.087	0.0760.112	0.760.76			
201	000	1	2094	2967.273	3204.319	1.00E-25	2.81E-23	9.702E-21	4504	4	0	0.064	0.0870.0780.1120.760.76					
300	000	1	1155	3190.171	3357.246	1.00E-25	2.55E-24	3.902E-22	450	4	4	0	0.065	0.086	0.084	0.111	0.760.76	
103	010	1	461	3273.600	3332.613	1. 01E-25	4.13E-25	9.687E-23	450	4	4	0	0.068	0.086	0.092	0.111	0.76	
004	010	1	14	3294.749	3331.276	1.03E-25	1.20E-25	2.51.535E-24	4504	4	0	0.072	0.082	0.0980.105	0.760.76			
310	010	1	3327.465	3327.465	1.06E-25	25.1.06E-25	25.1.06E-25	450	4	4	0	0.072	0.072	0.094	0.094	0.76		
013	000	1	1736	3595.887	3748.539	1. 01E-25	1.96E-23	6.146E-21	45033	0	0.065	0.0870.0790.1120.760.76						
112	000	1	485	3624.469	3762.052	1.00E-25	2.83E-24	1.383E-22	45033	0	0.065	0.081	0.081	0.1060.760.76				
004	000	1	681	3892.776	4060.783	1.00E-25	1.29E-23	5.741E-22	450	2	2	0	0.065	0.085	0.0880.1090.760.76			
310	000	1	1219	3894.373	4049.936	1.00E-25	7.90E-24	4.463E-22	450	2	2	0	0.065	0.0870.0880.1120.760.76				
103	000	1	2150	3912.153	4032.648	1.00E-25	4.33E-23	1.378E-20	450	2	2	0	0.064	0.0870.077	0.112	0.760.76		
N <sub>2</sub> O	( 4)																	
1310	0000	1	60	3046.220	3074.625	1.09E-24	2.73E-24	1.221E-22	466	1	1	1	0.0700.0890.085	0.1160.75	0.82			
0002	1000	1	58	3101.829	3154.201	1.03E-24	2.71E-24	1.144E-22	466	1	1	1	0.071	0.089	0.0860.116	0.75	0.82	
2110	0000	1	81	3162.794	3197.532	1.05E-24	7.12E-24	3.262E-22	466	1	1	1	0.0690.093	0.080	0.121	0.73	0.82	
0201	0000	2	59	3266.276	3320.368	1.05E-24	2.73E-24	1.183E-22	466	1	1	1	0.071	0.0890.0860.1160.75	0.82			
1111	0200	1	91	3280.070	3355.758	1. 01E-24	2.152E-23	7.431E-22	466	1	1	1	0.069	0.097	0.080	0.1270.73	0.82	
1111	0220	1	172	3280.981	3353.934	1. 01E-24	1.06E-23	1.016E-21	466	1	1	1	0.070	0.093	0.081	0.121	0.75	0.82
2111	0330	1	121	3281.457	3482.857	1. 01E-24	1.1	OE-23	5.725E-22	466	1	1	1	0.0700.090	0.081	0.1190.75	0.82	
0311	0110	1	260	3285.230	3383.462	1.02E-24	1.51E-22	1.506E-20	466	1	1	1	0.0690.0970.0770.127	0.73	0.82			
2111	0310	1	34	3288.513	3321.113	1. 01E-24	1.14E-24	3.649E-23	466	1	1	1	0.074	0.080	0.0970.105	0.75	0.77	
0201	0000	1	136	3295.982	3408.309	1.08E-24	1.65E-24	2.189.290E-20	466	1	1	1	0.069	0.097	0.0760.1270.73	0.82		
0201	0000	3	81	3296.447	3363.125	1.03E-24	7.52E-24	3.686E-22	466	1	1	1	0.070	0.093	0.082	0.121	0.75	0.82
0201	0000	4	82	3307.838	3373.540	1.02E-24	6.72E-24	2.332E-22	466	1	1	1	0.070	0.093	0.082	0.121	0.75	0.82
1201	1000	1	71	3310.979	3373.094	1.06E-24	4.51E-24	2.136E-22	466	1	1	1	0.0700.0900.083	0.1190.75	0.82			
0221	0000	1	82	3319.826	3414.419	1.04E-24	7.16E-24	3.204E-22	466	1	1	1	0.0690.0770.0770.101	0.730.82				
1001	0000	2	112	3370.824	3462.689	1.02E-24	1.15E-22	5.722E-21	466	1	1	1	0.069	0.0970.078	0.1270.73	0.82		
1001	0000	4	109	3378.948	3463.967	1.02E-24	5.82E-24	2.981E-21	466	1	1	1	0.0690.0970.0780.127	0.73	0.82			
1001	0000	3	115	3381.794	3473.528	1.04E-24	2.123E-22	6.218E-21	466	1	1	1	0.0690.0970.0770.127	0.73	0.82			
1111	0110	2	158	3382.909	3448.822	1.02E-24	6.92E-24	6.575E-22	466	1	1	1	0.0700.0970.0820.127	0.75	0.82			
2001	1000	1	112	3384.988	3476.512	1.02E-24	1.13E-22	5.624E-21	466	1	1	1	0.0690.0970.0780.127	0.730.82				
1001	0000	1	156	3386.212	3513.862	1.03E-24	3.31E-20	1.650E-18	466	1	1	1	0.0690.0970.070	0.1270.73	0.82			
1111	0110	1	338	3394.709	3506.679	1.03E-24	1.86E-21	11.854E-19	466	1	1	1	0.0690.0970.0760.127	0.730.82				
1111	0110	4	130	3396.960	3452.701	1.02E-24	3.42E-24	3.098E-22	466	1	1	1	0.0700.0890.085	0.1160.75	0.82			

Table 9 (continued)

SPECIES	1S0	#LINES	FMIN cm <sup>-1</sup>	FMAX cm <sup>-1</sup>	I MIN cm''' / (molecule x en('))	I MAX cm''' / (molecule x en('))	S-SUM	ACC RE	FPBHW	P MAX (cm <sup>-1</sup> /atm)	SELF	S MAX (cm <sup>-1</sup> /atm)	NTDP	N MAX (cm <sup>-1</sup> /atm)							
1111	0110	3	160	3397.027	3462.016	1.02E-24	6.90E-24	6.681E-22	466	1	1	1	0.070	0.0970.082	0.1270.75	0.82					
2111	1110	1	150	3398.949	3464.340	1.	01E-24	6.15E-24	5.793E-22	466	1	1	1	0.0700.090	0.083	0.1190.75	0.82				
1201	0200	1	111	3400.729	3492.494	1.11E-24	1.07E-22	5.346E-21	466	1	1	1	0.0690	0.0970.0780	0.1270.73	0.82					
2111	0001	1	31	3403.331	3440.339	1.	01E-24	1.42E-24	3.752E-23	466	1	1	1	0.073	0.083	0.094	0.110	0.75	0.79		
1221	0220	1	260	3403.821	3495.847	1.02E-24	1.03E-22	1.07E-20	466	1	1	1	0.0690	0.093	0.0780	0.121	0.73	0.82			
1001	0000	5	89	3411.522	3482.917	1.06E-24	1.22E-23	6.060E-22	466	1	1	1	0.0690	0.0970.081	0.1270.73	0.82					
0221	0310	1	148	3412.643	3477.046	1.03E-24	6.08E-24	5.703E-22	466	1	1	1	0.070	0.0900.083	0.1190.75	0.82					
0600	0000	3	5	3419.532	3461.685	1.12E-24	9.39E-24	2.805E-23	466	1	1	1	0.072	0.0730.094	0.094	0.790.80					
0600	0000	1	17	3428.066	3511.764	1.07E-24	4.1	OE-22	8.154E-22	466	1	1	1	0.069	0.070	0.0790.082	0.73	0.78			
0620	0000	1	13	3450.219	3503.988	1.28E-24	4.72E-22	9.133E-22	466	1	1	1	0.071	0.072	0.0870.094	0.800.82					
CH <sub>4</sub>	( 6 )																				
v6	GROUND	3	1406	970.390	1427.138	1.00E-26	1.75E-23	1.342E-21	3321516	0	0.080	0.080	0.090	0.090	0.75	0.75					
V 3	GROUND	3	561	1060.783	1438.420	1.03E-26	1.97E-23	9.498E-22	33215160	0.080	0.080	0.0900	0.0900	0.75	0.75						
V5	GROUND	3	1031	1262.749	1693.489	1.00E-26	3.83E-24	3.205E-22	332151600	0.080	0.080	0.0900	0.0900	0.75	0.75						
O <sub>2</sub>	( 7 )																				
xI	X0	1	146	1407.321	1705.6493	.68E-30	1.49E-28	6.159E-27	354	1	1	0	0.042	0.062	0.000	0.000	0.75	0.75			
NO	( 8 )																				
x3/2	1	x3/2	O	1	205	1733.303	1973.284	1.72E-26	3.34E-20	1.585	E-18	305	O	1	1	0.041	0.0670.054	0.0770.71	0.71		
x1/2	1	x1/2	O	1	212	1736.671	1971.9894	.45E-27	6.25E-20	2.997E-18	305	0	1	1	0.041	0.0690.054	0.0760.71	0.71			
NO <sub>2</sub>	( 10 )																				
001	000	1	3222	1538.182	1662.424	1.22E-23	2.56E-19	5.728E-	17454	44	1	1	0.0670	0.0670.0000.000	0.75	0.75					
020	000	1	155	1554.220	1653.517	2.97E-23	1.36E-21	6.825E-20	454	44	1	1	0.0670	0.0670.000	0.000	0.75	0.75				
011	010	1	802	1556.174	1639.205	1.05E-22	6.33E-21	1.198E-18	454	44	1	1	0.0670	0.0670.000	0.000	0.75	0.75				
HNO <sub>3</sub>	( 12 )																				
V5	00000000	1	19302	816.189	946.493	7.15E-24	1.29E-20	1.144E-17	444	999	0.110	0.110	0.300	0.300	0.75	0.75					
2W	00000000	1	18666	826.268	959.186	7.15E-24	8.69E-21	8.292	E-18	444	9990	0.1100	0.110	0.300	0.3000	0.75	0.75				
V 3	GROUND	1	20747	1098.376	1387.849	1.00E-23	3.35E-20	2.712	E-17	000	77	1	0.1100	0.1100.000	0.0000	0.75	0.75				
V8+V9	GRWND	1	6214	1165.014	1232.483	1.61E-23	1.58E-21	1.199E-18	00066	1	0.1100	0.1100.0000	0.000	0.75	0.75						
V4	GROUND	1	19082	1229.867	1387.561	1.11E-23	2.00E-20	1.366E-17	000	78	1	0.1100	0.110	0.0000	0.000	0.75	0.75				
V2	GROUND	1	21946	1650.014	1769.982	2.12E-24	4.24E-20	4.381E-17	000	1	1	1	0.110	0.1100.0000	0.000	0.75	0.75				
HF	( 14 )																				
1	0	1	29	3269.779	4368.140	1.15E-26	2.37E-18	1.572	E-17	462	2	1	2	0.0100	0.105	0.075	0.7290.22	1.00			
HCl	( 15 )																				
1	1	2	12	20.240	239.339	1.01	E-263	.95E-25	2.220E-24	482	1	1	1	0.009	0.089	0.080	0.245	0.290.76			
1	1	1	13	20.270	258.994	1.98E-26	1.23E-24	6.902E-24	482	1	1	1	0.0100	0.0970	0.075	0.264	0.290.76				
0	0	2	21	20.847	418.7384	.42	E-264	.63E-19	2.585E-18	582	1	1	1	0.005	0.0890	0.050	0.245	0.290.76			
0	0	1	22	20.878	437.392	1.95E-26	1.45E-18	8.096E-18	582	1	1	1	0.010	0.0970	0.050	0.264	0.29	0.76			
1	0	2	38	2398.957	3151.461	1.22E-26	61.61E-19	1.518E-18	472	2	1	1	0.005	0.0890	0.0500	0.253	0.130.76				
1	0	1	39	2400.278	3160.444	1.81E-26	5.03	E-194	.749E-18	472	2	1	1	0.005	0.0890	0.0500	0.253	0.13	0.76		
2	1	1	21	2554.264	2962.536	1.43	E-267	.7149E-24	472	1	1	1	0.013	0.0890	0.085	0.253	0.13	0.76			
2	1	2	19	2577.751	2947.382	1.15E-26	2.49E-25	2.382E-24	472	1	1	1	0.0160	0.0890	0.0220	0.253	0.13	0.76			
2	0	1	35	5159.439	5829.709	2.29E-26	1.18E-20	1.077E-19	462	1	1	1	0.005	0.0980	0.055	0.253	0.13	0.76			
2	0	2	33	5194.557	5825.543	3.71E-26	3.76E-21	3.434E-20	462	1	1	1	0.005	0.0890	0.055	0.253	0.130.76				
3	1	1	13	5321.585	5568.350	1.13E-26	3.22E-26	2.738E-25	462	1	1	1	0.033	0.0890	0.154	0.253	0.35	0.76			
3	1	2	2	5510.529	5525.897	1.03E-26	1.04E-26	2.068E-26	462	1	1	1	0.062	0.072	0.2370.245	0.71	0.72				
3	0	1	29	7895.987	8454.457	1.12E-26	8.09E-23	7.180E-22	352	1	1	1	0.0060	0.0890	0.065	0.2530	0.130.76				
3	0	2	27	7933.979	8448.539	1.36E-26	2.58E-23	2.288E-22	352	1	1	1	0.0070	0.0890	0.070	0.2530.05	0.76				
ClO	( 18 )																				
X1/2	1	x1/2	o	2	190	770.401	875.322	1.06E-24	2.17E-22	1.641	E-20	442	1	1	1	0.093	0.093	0.0000	0.0000.75	0.75	
X3/2	1	x3/2	O	2	226	773.840	878.516	1.21E-24	1.03E-21	7.841E-20	442	1	1	1	0.093	0.093	0.000	0.000	0.75	0.75	
x1/2	1	x1/2	o	1	204	776.285	882.	995	1.11E-24	6.83E-22	5.117E-20	442	1	1	1	0.093	0.093	0.0000	0.0000.75	0.75	
x3/2	1	x312	O	1	236	779.760	886.215	1.18E-24	3.24E-21	2.444	E-19	442	1	1	1	0.0930	0.0930	0.000	0.000	0.75	0.75

Table 9 (continued)

SPECIES	ISO	#LINES	FMIN	FMAX	I MIN	1 MAX	s- SUM	ACC	REF	PBHU	PMAX	SELF	SMAX	NTDP	NMAX
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>'''</sup>	(molecule x cm <sup>-2</sup> )				(cm <sup>-1</sup> /atm)	(cm <sup>-1</sup> /atm)				
OCS	(19)														
0110	0000	1	209	493.260	549.975	3.76E-23	4.53E-213.421E-19	521	1	1	1	0.082	0.1090.1160.1690.300.90		
1000	0000	1	160	822.740	887.377	1.42E-221.55E-20	1.109E-18	531	1	3	1	0.082	0.109	0.113	0.1690.30
0200	0000	1	160	1018.894	1083.744	4.88E-23	5.22E-213.757E-19	531	1	4	1	0.0820.1090.113	0.1690.30	0.90	
2000	0000	1	140	1676.692	1733.200	1.07E-222.92E-212.097E-19	521	1	1	1	0.082	0.1090.1160.1690.300.90			
1200	0000	1	160	1860.771	1925.538	4.38E-233.67E-212.697E-19	521	2	5	1	0.082	0.1090.113	0.1690.30	0.90	
1310	0110	1	276	1863.083	1920.944	2.75E-23	6.21E-228.977E-20	521	2	5	1	0.082	0.1060.1160.1690.300.90		
0001	0000	3	159	1970.284	2034.044	1.30E-221.16E-208.421E-19	991	99	1	0.082	0.109	0.113	0.169	0.30	0.90
0001	0000	1	220	2003.194	2091.720	5.51E-231.19E-188.579E-17	521	2	5	1	0.000	0.1090.0000.1690.000.90			
0111	0110	1	356	2008.832	2081.552	1.67E-228.56E-201.230E-17	521	2	5	1	0.082	0.1060.113	0.1690.30	0.90	
0001	0000	2	159	2022.958	2085.346	5.55E-224.40E-203.216E-18	991	99	1	0.082	0.1090.113	0.1690.300.90			
0400	0000	1	140	2082.385	2139.251	1.45E-225.68E-213.927E-19	521	2	5	1	0.0820.1090.1160.169	0.300.90			
0510	0110	1	236	2093.757	2143.976	7.00E-237.31E-229.976E-20	521	25	1	0.082	0.1060.120	0.1690.300.90			
3000	0000	1	140	2518.644	2575.061	6.79E-241.56E-221.140E-20	521	25	1	0.082	0.1090.1160.1690.300.90				
0111	0000	1	209	2542.361	2598.907	7.83E-257.83E-235.691E-21	531	2	2	1	0.0820.1090.1160.169	0.30	0.90		
2200	0000	1	140	2701.118	2757.748	6.60E-241.59E-221.160E-20	521	2	5	1	0.082	0.1090.1160.1690.300.90			
1111	0110	1	316	2860.425	2925.128	1.20E-231.02E-211.497E-19	521	2	5	1	0.082	0.1060.113	0.1690.30	0.90	
1001	0000	1	180	2867.400	2939.850	3.43E-231.26E-209.255E-19	521	2	5	1	0.082	0.1090.113	0.1690.30	0.90	
1400	0000	1	140	2912.288	2969.087	1.49E-241.62E-221.044E-20	521	25	1	0.082	0.1090.1160.1690.300.90				
0201	0000	1	160	3059.953	3124.613	1.04E-239.41E-226.868E-20	521	2	5	1	0.082	0.109	0.113	0.169	0.30
0311	0110	1	276	3063.233	3120.931	6.00E-241.41E-222.029E-20	521	2	5	1	0.0820.1060.1160.169	0.300.90			
0002	0000	1	160	4053.648	4117.994	7.56E-237.90E-215.718E-19	521	1	1	1	0.082	0.1090.1130.1690.300.90			
HOC <small>l</small>	(21)														
001	000	1	845	679.018	757.953	5.38E-234.95E-211.273E-18	331	1	1	0	0.060	0.0600.0000.0000.75	0.75		
001	000	2	530	679.476	755.946	4.63E-234.82E-216.904E-19	331	1	1	0	0.060	0.060	0.000	0.0000.75	0.75
010	000	1	611	1180.966	1249.953	1.47E-223.17E-204.901E-18	331	1	1	0	0.0600.0600.0000.000	0.75	0.75		
010	000	2	523	1185.936	1249.946	1.55E-221.03E-201.644E-18	331	1	1	0	0.060	0.060	0.000	0.000	0.75
CH <sub>3</sub> Cl	(30)														
V3	GROUND	2	1752	661.793	765.094	1.01E-233.67E-219.715E-19	351	1	1	0	0.080	0.080	0.000	0.0000.75	0.75
V3	GROUND	1	1993	666.344	771.445	1.00E-231.13E-202.960E-18	351	1	1	0	0.080	0.080	0.000	0.000	0.75
C <sub>2</sub> H <sub>6</sub>	(38)														
V9	GROUND	1	10000	745.225	951.650	6.88E-271.03E-216.967E-19	331	1	1	1	0.100	0.100	0.0000.000	0.75	0.75
C <sub>2</sub> H <sub>4</sub>	(40)														
00011110	00000000	1	119	1192.333	1469.865	1.37E-271.38E-192.664E-18	000	1	1	1	0.0400.1160.110	0.162	0.75	0.75	
01011110	00000000	1	63	3204.731	3351.912	2.22E-212.46E-194.961E-18	460	2	2	1	0.045	0.1160.1100.162	0.75	0.75	
00100000	00000000	1	62	3211.602	3358.285	8.93E-222.22E-194.355E-18	4602	2	1	0.043	0.1160.1100.162	0.75	0.75		
HDO	(49)														
000	000	1	461	0.007	100.490	1.24E-321.27E-222.585E-21	00000	0	0	0.0080.103	0.000	0.0000.64	0.64		
010	000	1	1653	1104.970	1894.299	1.00E-272.67E-232.816E-21	000	0	0	0.008	0.103	0.000	0.000	0.64	0.64
010	000	2	200	1231.680	1607.611	1.00E-267.94	E-265.832E-24443	77	0	0.031	0.105	0.0000.000	0.75	0.75	
100	000	1	1333	2332.099	3132.932	1.01E-279.75E-24	6.337E-2200000	0	0	0.0080.103	0.0000.0000.64	0.64			
020	000	1	953	2486.140	3361.318	1.00E-271.23E-24	8.468E-23000	0	0	0.00080.103	0.000	0.000	0.64	0.64	
001	000	1	1651	3236.354	4121.496	1.01E-271.75E-231.416E-21	000	000	000	0.0080.103	0.0000.0000.64	0.64			
110	000	1	860	3843.445	4496.503	1.00E-279.36E-256.426E-23	000	0	0	0.019	0.103	0.000	0.000	0.64	0.64
030	000	1	602	3879.178	4639.031	1.01E-278.76E-253.504E-23	00000	0	0	0.024	0.103	0.000	0.000	0.64	0.64
011	000	1	576	4850.495	5384.821	3.01E-275.53E-253.671E-23	000	0	0	0.0190.103	0.000	0.000	0.64	0.64	
200	000	1	216	5154.643	5507.548	3.07E-272.94E-251.589E-23	000	0	0	0.029	0.103	0.000	0.000	0.64	0.64

Table 10

## Summary of the 1995 Supplemental Linelist

SPECIES	ISO	#LINES	FMIN cm <sup>-1</sup>	FMAX cm <sup>-1</sup>	I <sub>MIN</sub> (cm <sup>-1</sup> /molecule x cm <sup>-2</sup> )	I <sub>MAX</sub> (cm <sup>-1</sup> /molecule x cm <sup>-2</sup> )	S-SUM	ACC	REF	PBHW	PMAX	SELF	SMAX	NTDP	NMAX
O <sub>2</sub>	( 7)														
xI	Xo	1	162	1432.508	1676.962	5.14E-33	4.41E-29	1.470	E-27	344	2	2	0	0.042	0.062
HNO <sub>3</sub>	(12)														
3V9	V9	1	4780	845.111	908.834	8.14E-23	2.78E-21	2.030E-18	000	0	0	0	0.110	0.110	0.000
V5+V9	V9	1	3971	847.611	904.221	8.13E-23	1.70E-21	1.216E-18	000	0	0	0	0.110	0.110	0.000
H <sub>2</sub> CO	(20)														
010001	000000	1	587	1707.093	1781.387	3.00E-22	5.98E-20	7.195E-18	000	0	0	0	0.100	0.100	0.000
HO <sub>2</sub>	(22)														
001	000	1	1146	1032.068	1144.963	1.00E-23	6.80E-21	1.247E-18	000	0	0	0	0.080	0.080	0.100
000	000	1	2372	1055.186	1454.546	4.41E-23	2.89E-20	1.394E-17	000	0	0	0	0.100	0.100	0.000
010	000	1	1229	1145.513	1459.718	1.01E-23	1.11E-20	2.077E-18	000	0	0	0	0.080	0.080	0.100
100	000	1	2073	3202.033	3675.819	1.00E-23	3.08E-21	6.847E-19	000	0	0	0	0.080	0.080	0.100
HONO	(24)														
000000	1	2348	779.126	1711.707	1.39E-22	2.76E-20	2.059E-17	000	0	0	0	0.100	0.100	0.000	0.000
HO <sub>2</sub> NO <sub>2</sub>	(25)														
V4	00000000	1	341	802.478	803.654	6.75E-24	5.98E-21	9.140E-19	000	0	0	0	0.100	0.100	0.000
N <sub>2</sub> O <sub>5</sub>	(26)														
V3	GROUND	1	401	725.000	765.000	1.18E-20	2.03	E-193	.674E-17	000	0	0	0.800	0.8000	0.000
GROUND	1	360	1221.886	1269.014	7.57E-22	3.79E-19	4.677E-17	000	0	0	0	0	7.50025	0.000	0.000
VI	GRWNO	1	2739	1671.050	1807.950	3.56E-22	1.42E-19	1.639E-16	000	0	0	0	0.020	0.00020	0.000
C10NO <sub>2</sub>	(27)														
V9	1	6411	763.641	797.741	1.25E-24	4.98E-22	9.191E-19	000	0	492	0.140	0.140	0.800	0.800	0.75
V4	GROUND	2	6208	765.212	790.805	6.41E-25	2.52E-22	4.656E-19	000	0	492	0.140	0.140	0.800	0.800
V4	GROUND	1	6970	766.150	792.488	3.87E-24	7.70E-22	1.439E-18	00000	492	0.140	0.140	0.800	0.8000	0.75
V2	GROUND	1	3675	1270.007	1309.991	2.00E-24	2.03E-20	2.831E-17	000	0	0	0	0.030	0.100	0.000
CH <sub>3</sub> F	(29)														
VI	GROUND	1	739	987.918	1089.135	5.41E-23	1.16E-19	1.806E-17	000	0	0	0	0.100	0.100	0.000
CH <sub>3</sub> Cl	(30)														
V2	GRWND	1	513	1324.697	1377.725	5.06E-23	6.16E-21	1.057E-18	000	0	0	0	0.100	0.100	0.000
V5	GROUND	2	61	1458.986	1459.770	5.43E-24	1.05E-21	2.714E-20	000	0	0	0	0.080	0.080	0.300
V5	GROUND	1	47	1459.218	1460.144	1.78E-23	3.12E-21	7.940E-20	000	0	0	0	0.080	0.080	0.300
CCl <sub>2</sub> F <sub>2</sub>	(32)														
REG1ON	1	381	920.038	924.202	5.22E-21	5.98E-20	8.285E-18	000	0	0	0	0	0.055	0.055	0.000
V1 REGION	1	5179	1070.038	1129.996	3.52E-25	2.55E-20	4.580E-17	000	0	0	0	0	0.030	0.030	0.000
v8 REG1ON	1	593	1147.277	1161.2794	.23E-23	1.04	E-195	.851E-18	000	0	0	0	0.030	0.030	0.000
CCl <sub>3</sub> F	(33)														
V4 REG1ON	1	842	833.500	860.500	4.55E-22	1.52E-18	6.119E-17	000	0	0	0	0.100	5.000	0.000	0.000
V1 REGION	1	3651	1060.004	1099.9986	5.56E-22	1.55E-20	2.421E-17	000	0	0	0	0.030	0.0300	0.000	0.75
CH <sub>3</sub> CCl <sub>3</sub>	(34)														
V2 Q BRANCH	1	251	1382.500	1385.000	6.97E-24	2.07E-21	1.250E-19	000	0	0	0	0.100	0.100	0.000	0.000

Table 10 (continued)

Table 11 Revisions to be taken from HITRAN 1995

Species	Anticipated Update
CO*	Revised intensities
O <sub>3</sub>	default values for pressure shifts
NO	hot bands at 5.1 $\mu\text{m}$
NO <sub>2</sub>	prediction of bands at 6 $\mu\text{m}$
NH <sub>3</sub>	new bands at 4, 3, 2.3 and <u>2 <math>\mu\text{m}</math></u>
HNO <sub>3</sub>	new hot bands at 11 $\mu\text{m}$
CH <sub>3</sub> Cl	air-broadened widths
COF <sub>2</sub>	revised prediction of $\nu_4$ region
C <sub>2</sub> H <sub>2</sub>	$\nu_5$ at 14 $\mu\text{m}$ region
H <sub>2</sub> S	$\nu_1, \nu_3$ and $2\nu_2$ at 4 $\mu\text{m}$ ,

Table 12 Estimated Intensity Uncertainties in Regions Used by ATMOS

Species	Region (cm-l)	%acc. (2σ)	Recommendations / comments
H <sub>2</sub> O	1380-1980	4	
	2960-3300	4	
HDO	1420-1515	5	
H <sub>2</sub> <sup>18</sup> O	1415-1690	5	
H <sub>2</sub> <sup>17</sup> O	1455-1776	5	
CO <sub>2</sub>	650- 960	4	
	1910-2400	3	/may bc 2%
	3205-3630	3	/may bc 2%
<sup>12</sup> C <sup>18</sup> O <sup>16</sup> O	1230-1385	5	
D <sub>3</sub>	770-3170	4	
D <sub>3</sub> -686	980-1000	10	
O <sub>3</sub> - 668	1090-1091	20	higher cm-l should bc improved and abundance assumptions should bc checked for both 668 and 686
N <sub>2</sub> O	1150-3460	3	/may bc 2%
CO	2070-2200	3	/may bc 2%
CH <sub>4</sub>	1230-4315	3	
CH <sub>3</sub> D	2950-3100	20	complete analysis needed
NO	1840-1920	3	
NO <sub>2</sub>	1580-1640	4	
	2915-2925	6	
HNO <sub>3</sub>	865-1730	15	hot bands needed
HF	3790-4140	3	
HCl	27.30-2980	3	
OCS	<b>2040-2055</b>	<b>8</b>	
HNO <sub>4</sub>	<b>801- 805</b>	20	need data more /cross sections at 220K only
N <sub>2</sub> O <sub>5</sub>	1210-1260	15	
C1ONO <sub>x</sub>	779- 781	20	hot bands needed
HCN	3270-3360	4	
CH <sub>3</sub> Cl	2966-2968	10	complete prediction needed / only partial list
CF <sub>4</sub>	12.82-1285	10	
CCl <sub>2</sub> F <sub>2</sub>	<b>920- 940</b>	8	
CCl <sub>3</sub> F	<b>830- 870</b>	10	
CCL	776- 783	20	
COF <sub>2</sub>	772-774.1936-1940	10	
C <sub>2</sub> H <sub>6</sub>	2976-2977	10	complete prediction needed / only partial list
C <sub>2</sub> H <sub>2</sub>	755- 776	6	
CHClF <sub>2</sub>	828- 829	10	
SF <sub>6</sub>	945- 952	10	/linelist on 1992 HITRAN should bc removed

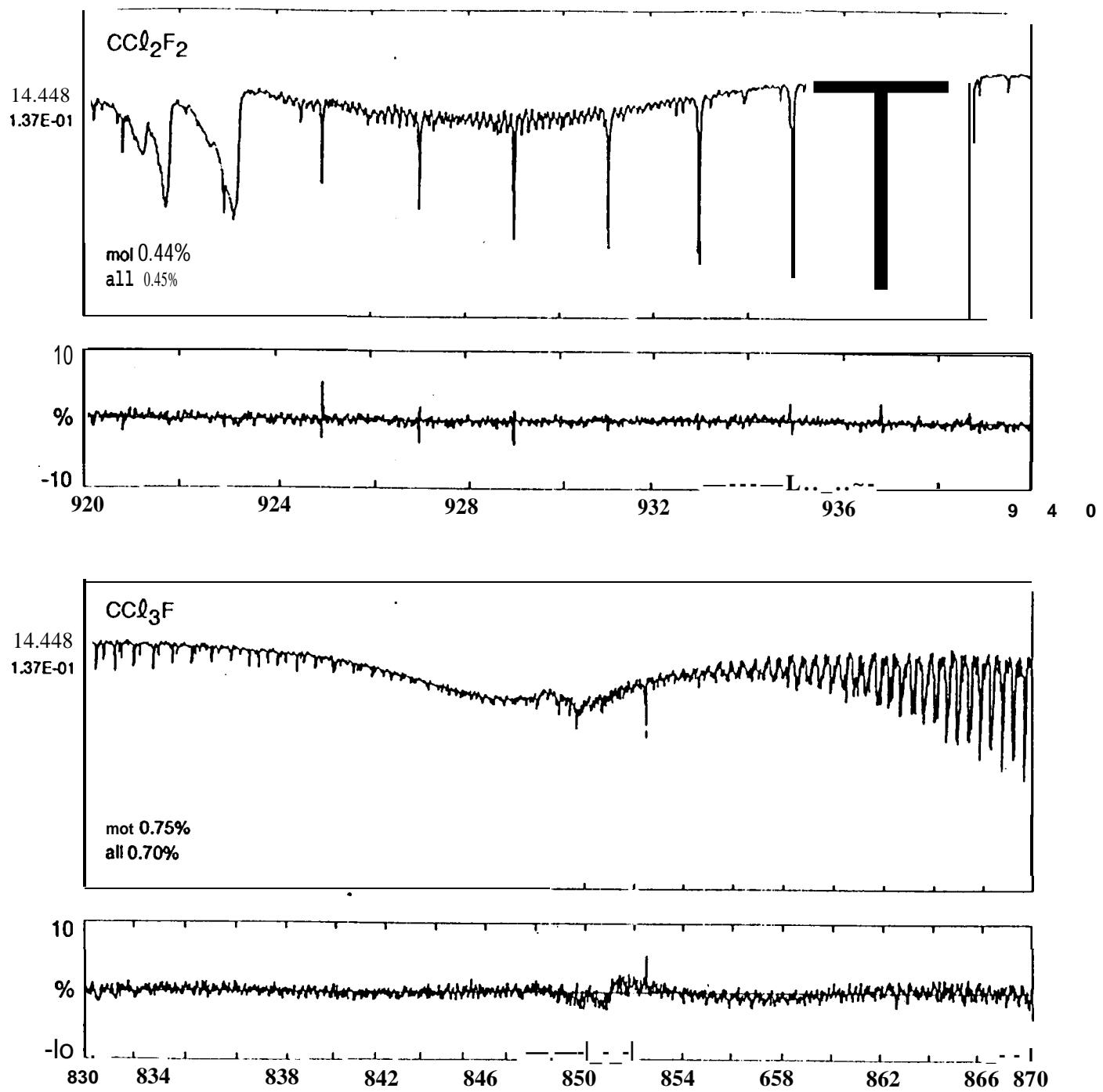


Fig. 1 Modelling the atmospheric absorption of CFC-12 (top) and CFC-11 (bottom) in ATMOS data using laboratory cross sections [14-16]. The tangent altitude is 14.4 km. The Q and R branches of the  $\text{CCl}_2\text{F}_2$  band at  $924\text{-cm}^{-1}$  are overlapped by the strong  $\text{CO}_2$  transitions. The R branch of the  $\text{CCl}_3\text{F}$  band near  $850\text{ cm}^{-1}$  is overlapped by manifolds of  $\text{HNO}_3$  between  $856$  and  $870\text{ cm}^{-1}$  while the Q branch is overlapped by weak  $\text{CO}_2$  and  $\text{O}_3$  transitions.